CIVIL-557
Decision-Aid Methodologies in Transportation
Lecture IV
Metaheuristics

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Outline

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What is a heuristic?

"A heuristic is a problem-solving strategy that uses practical and common-sense approaches to find solutions that may **not be optimal** *but are* **good enough** *for the given situation. It is a* **rule of thumb** *or an* **educated guess** *that is used when an exact or optimal solution is* **difficult or impossible** *to find."*

Why use a heuristic?

Different reasons may lead one to choose a heuristic:

- A solution is required rapidly, within a few seconds or minutes. The instance is so large and/or complicated that it cannot be formulated as an IP or MIP of reasonable size.
- Even though it has been formulated as an MIP, it is difficult or impossible for the branch-and-bound algorithm to find good feasible solutions.
- For certain combinatorial problems such as vehicle routing and machine scheduling, it is easy to find feasible solutions by inspection or knowledge of the problem structure. However, a general-purpose mixed-integer programming approach is ineffective.

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Greedy Algorithms

- Greedy heuristics construct a solution incrementally, starting with an empty solution and selecting the item with the best immediate benefit at each step.
- Greedy heuristics are simple and efficient, but may not always find the optimal solution.
- Greedy heuristics can be based on different criteria for selecting the "best" item at each step that minimizes cost.
- Greedy heuristics can be modified or combined with other methods, such as local search, to improve the solution.
- The effectiveness of a greedy heuristic depends on the problem structure and the quality of the criteria used to select the items at each step.

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Nearest Neighbor Heuristic

- It is a **greedy** heuristic that builds a solution iteratively;
- The nearest neighbor algorithm begins by selecting a current city randomly.
- The algorithm selects the nearest unvisited city to the current city at each step, until all cities are visited;
- It has a time complexity of $\mathcal{O}(n^2)$;
- The nearest neighbor heuristic is classified as a **construction** heuristic that builds a solution from scratch.

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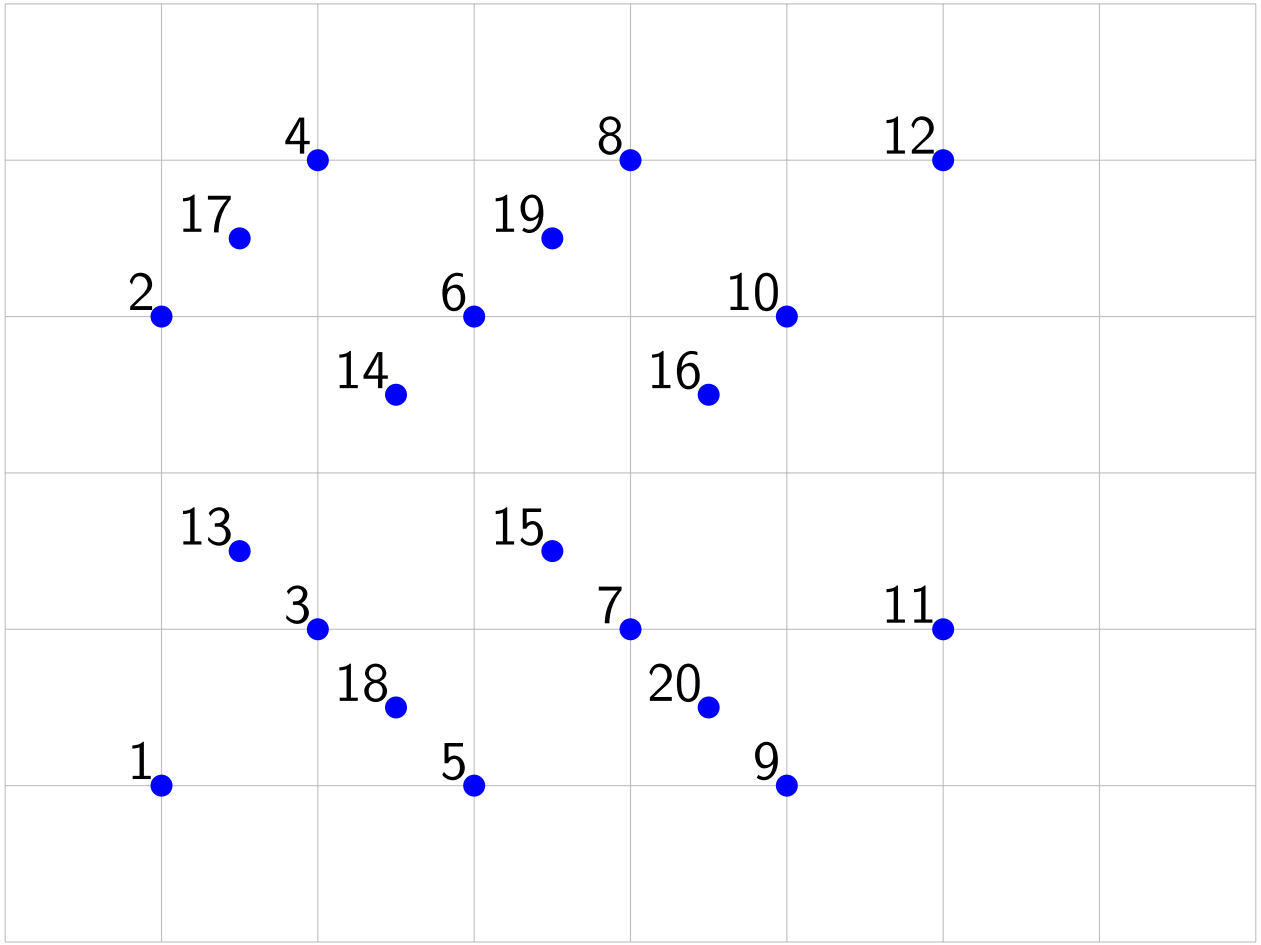
Nearest Neighbor Heuristic

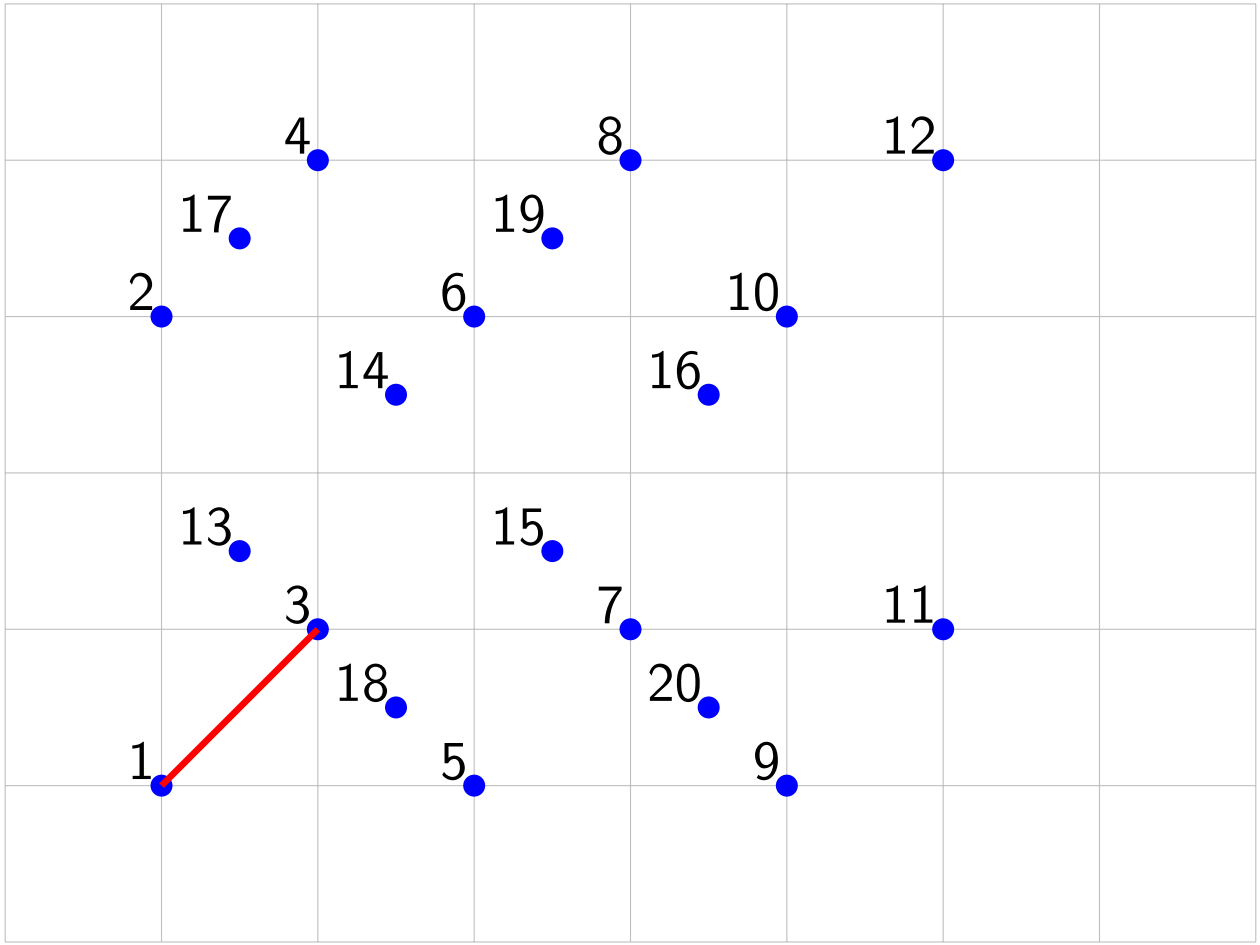
Input: A set of N cities, their pairwise distances, and a starting city s
Output: A tour of the cities

$s_{current} \leftarrow s$;
while *there are unvisited cities* **do**
    for *j in Unvisited* **do**
        Find the nearest neighbor of $s_{current}$;
        Let j^* be the unvisited city closest to $s_{current}$;
        Add the edge $(s_{current}, j^*)$ to the tour;
        $s_{current} \leftarrow j^*$;
    end
end
Add the edge $(s_{current}, s)$ to complete the tour;
return the resulting tour;

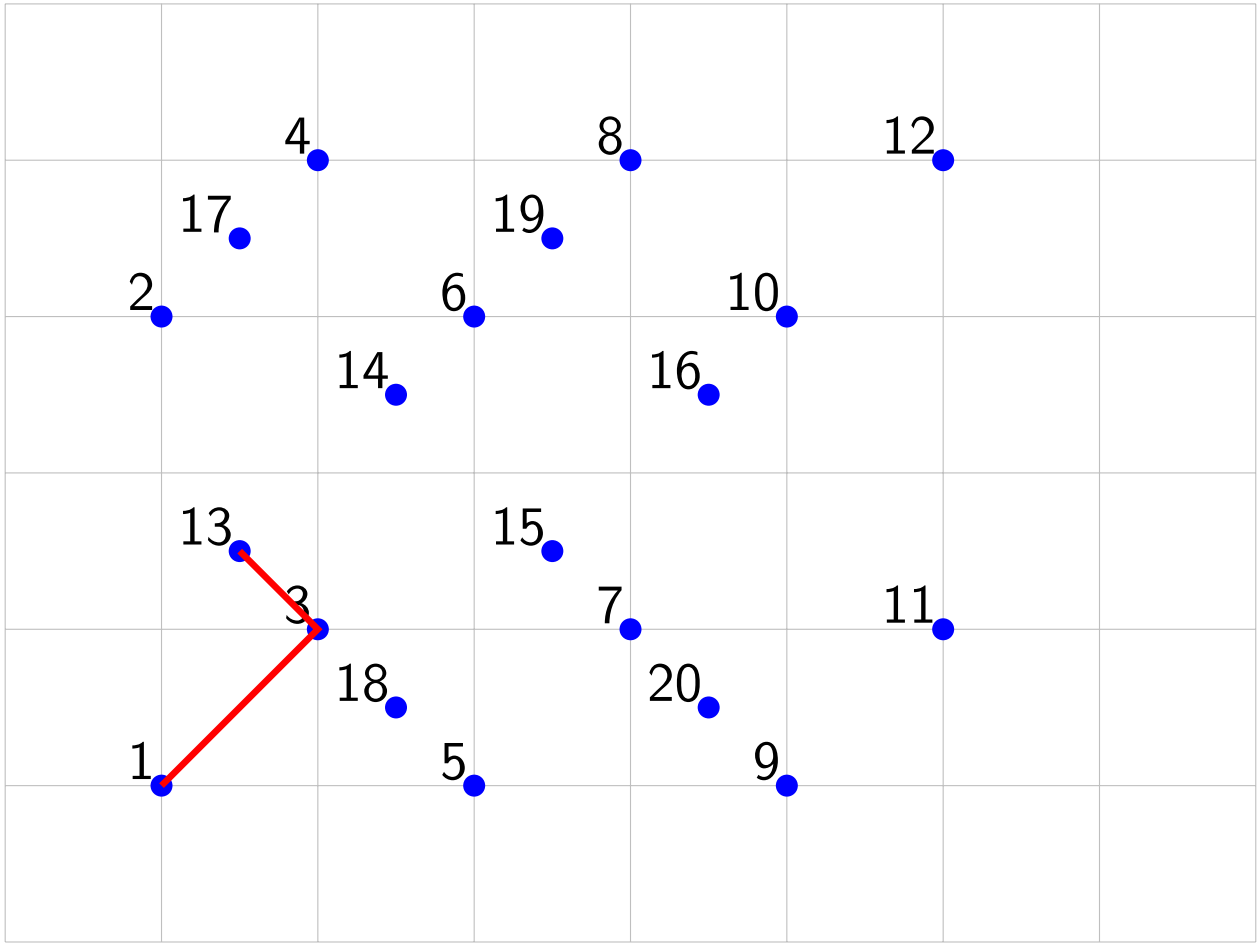
Nearest Neighbor Example



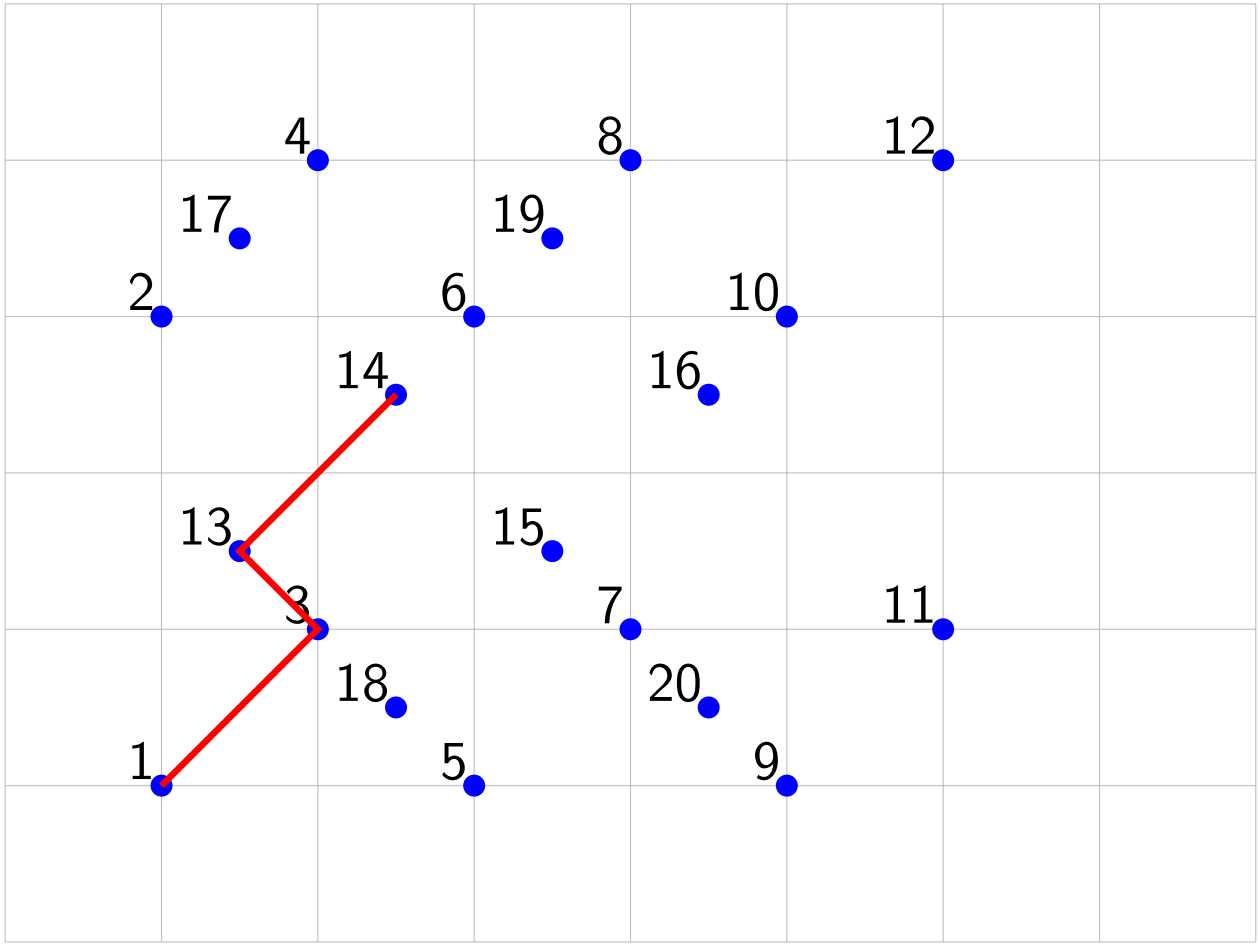
Nearest Neighbor Example



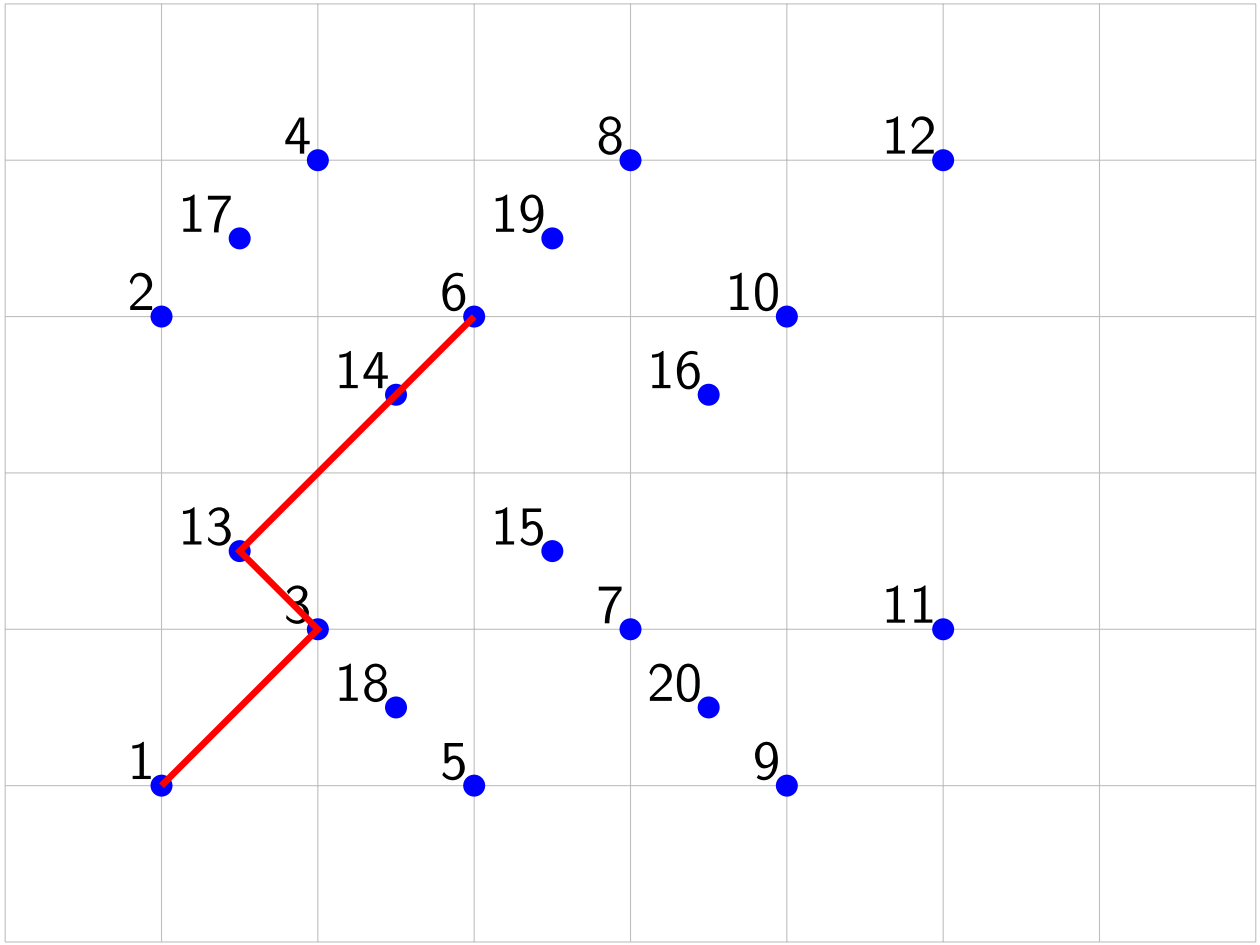
Nearest Neighbor Example



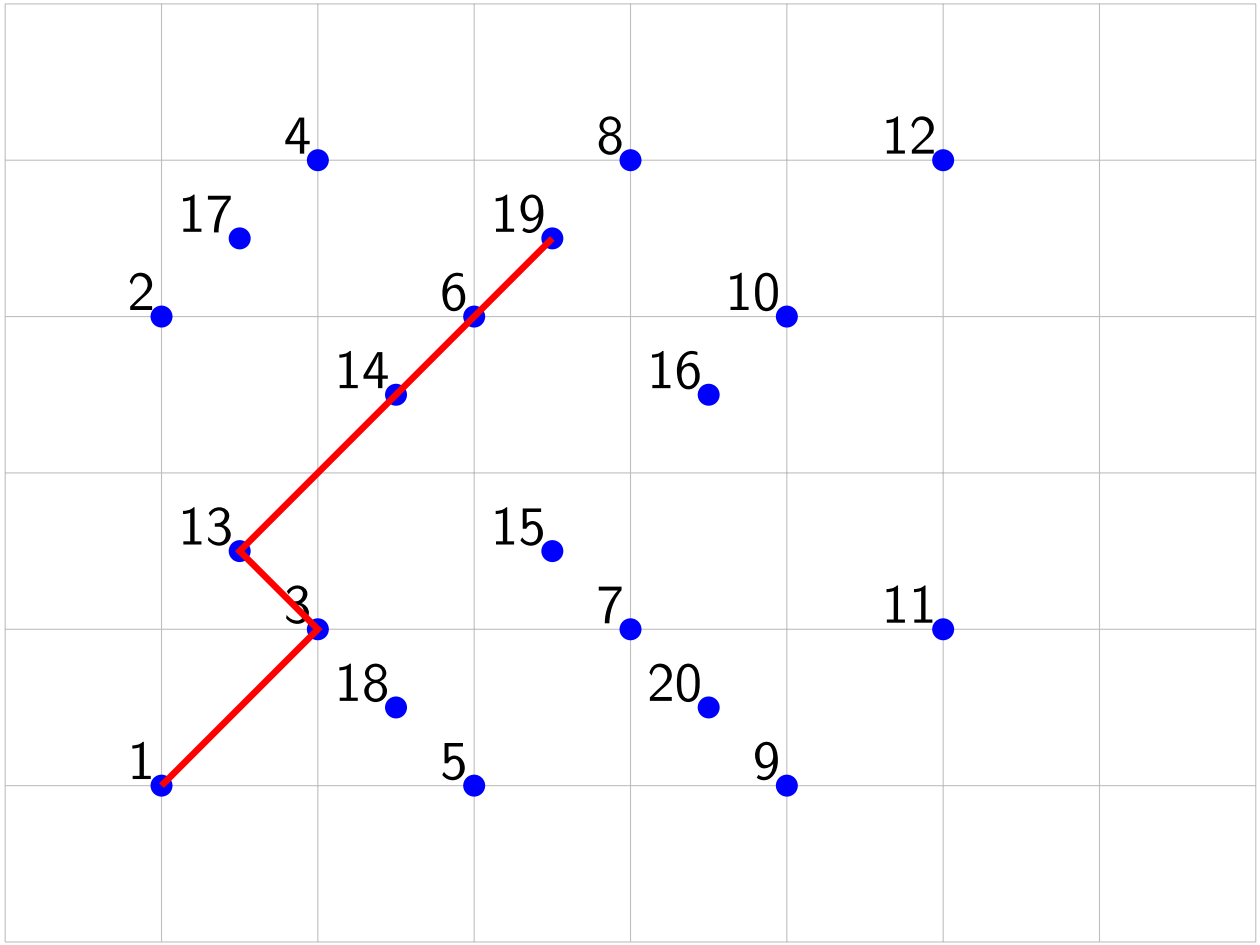
Nearest Neighbor Example



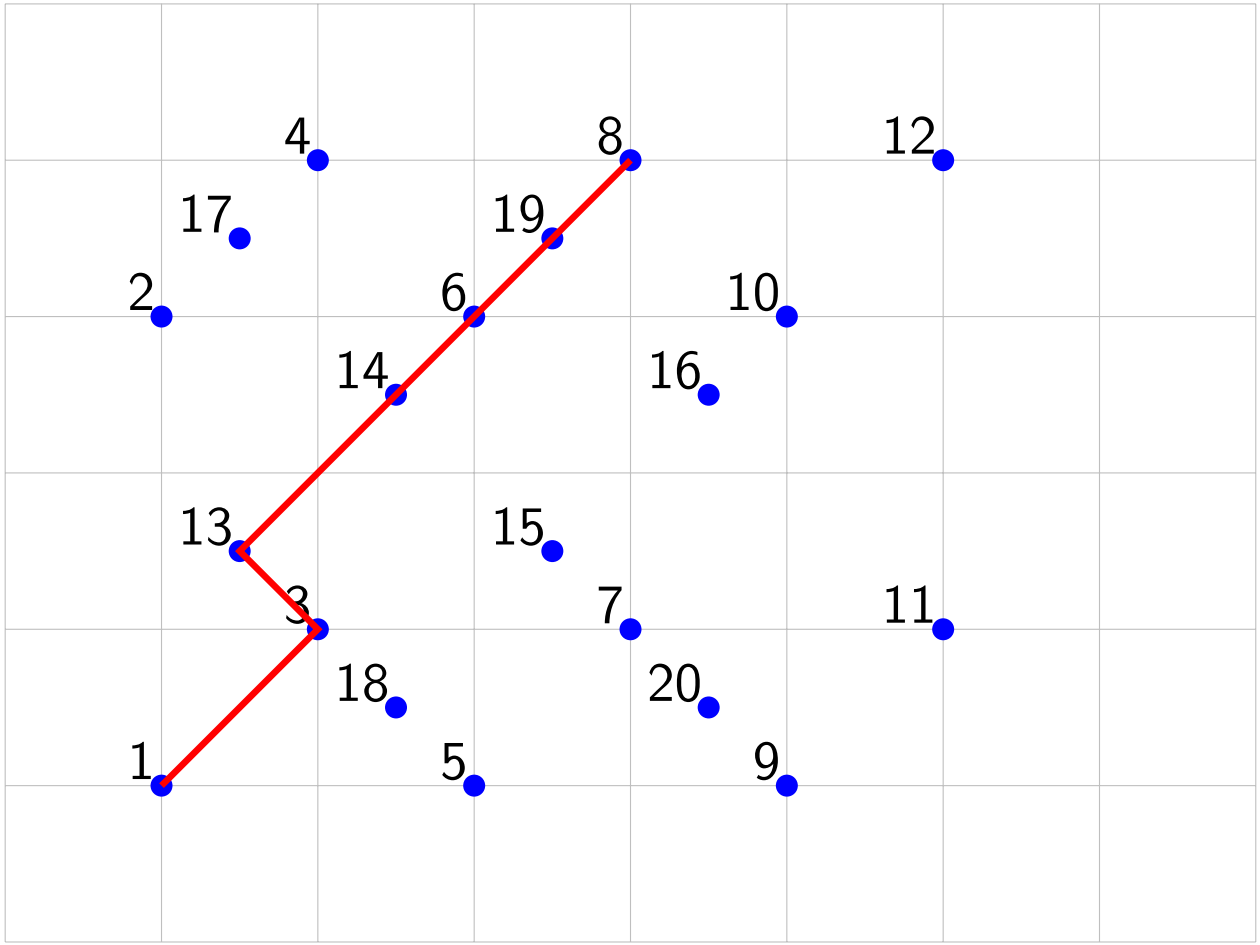
Nearest Neighbor Example



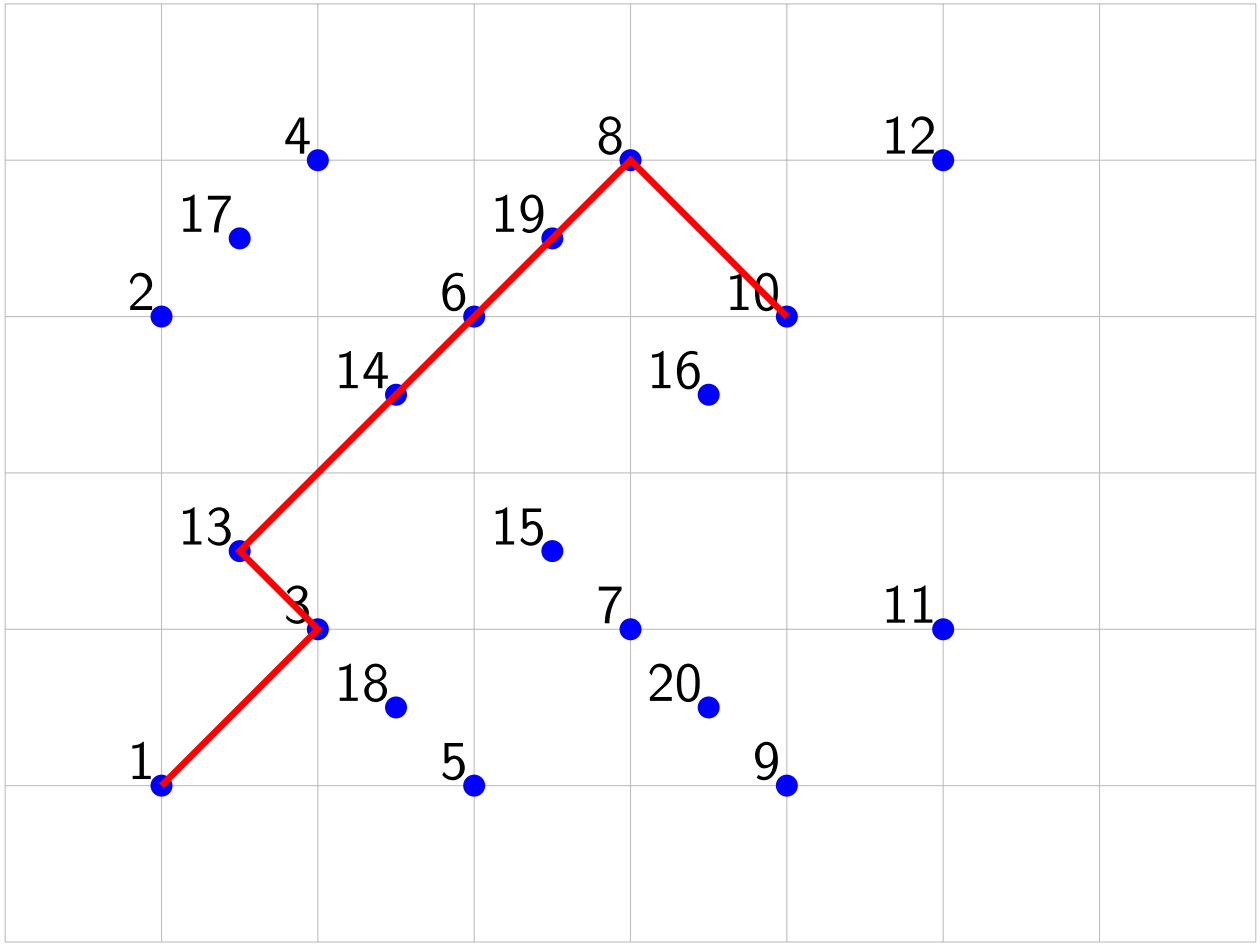
Nearest Neighbor Example



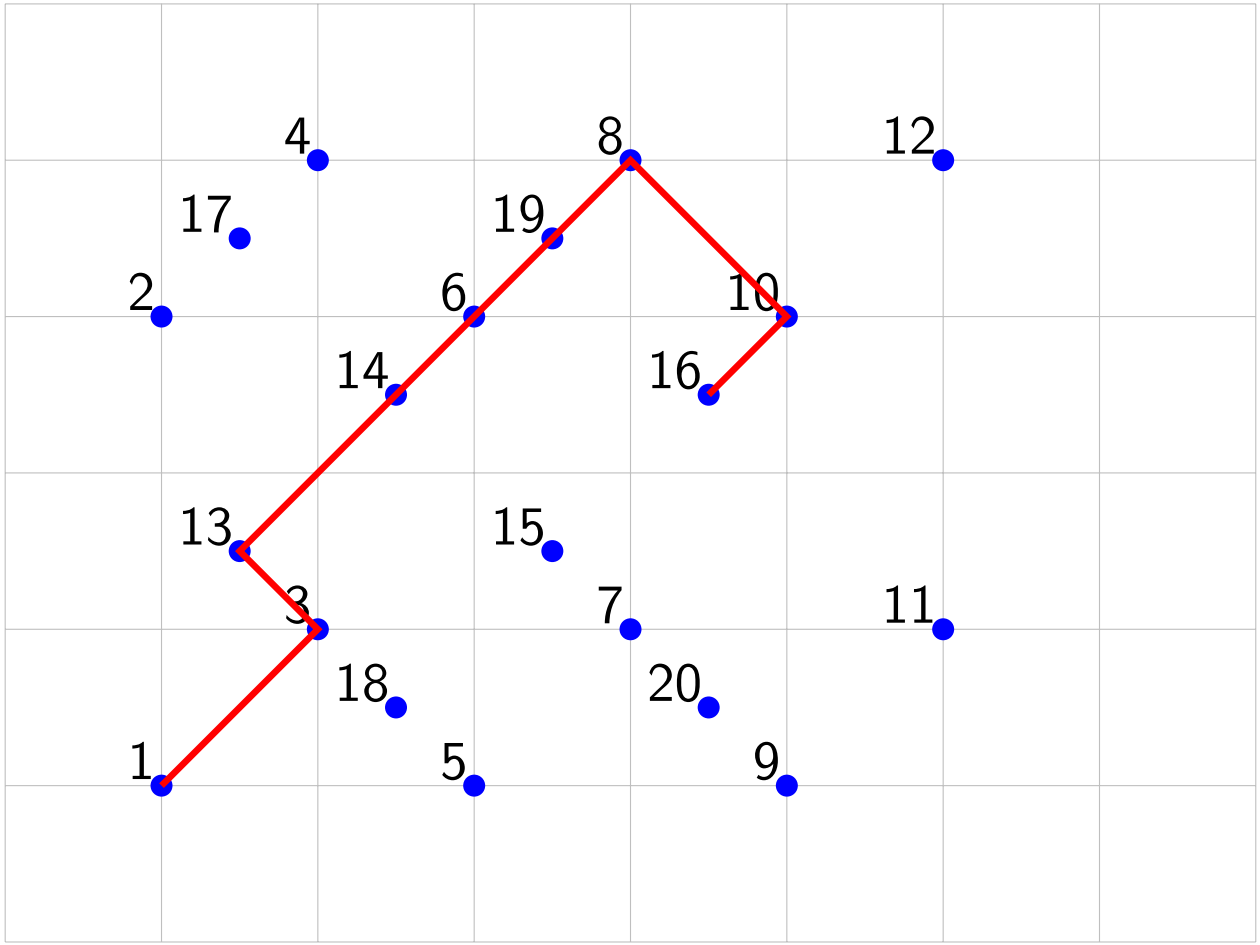
Nearest Neighbor Example



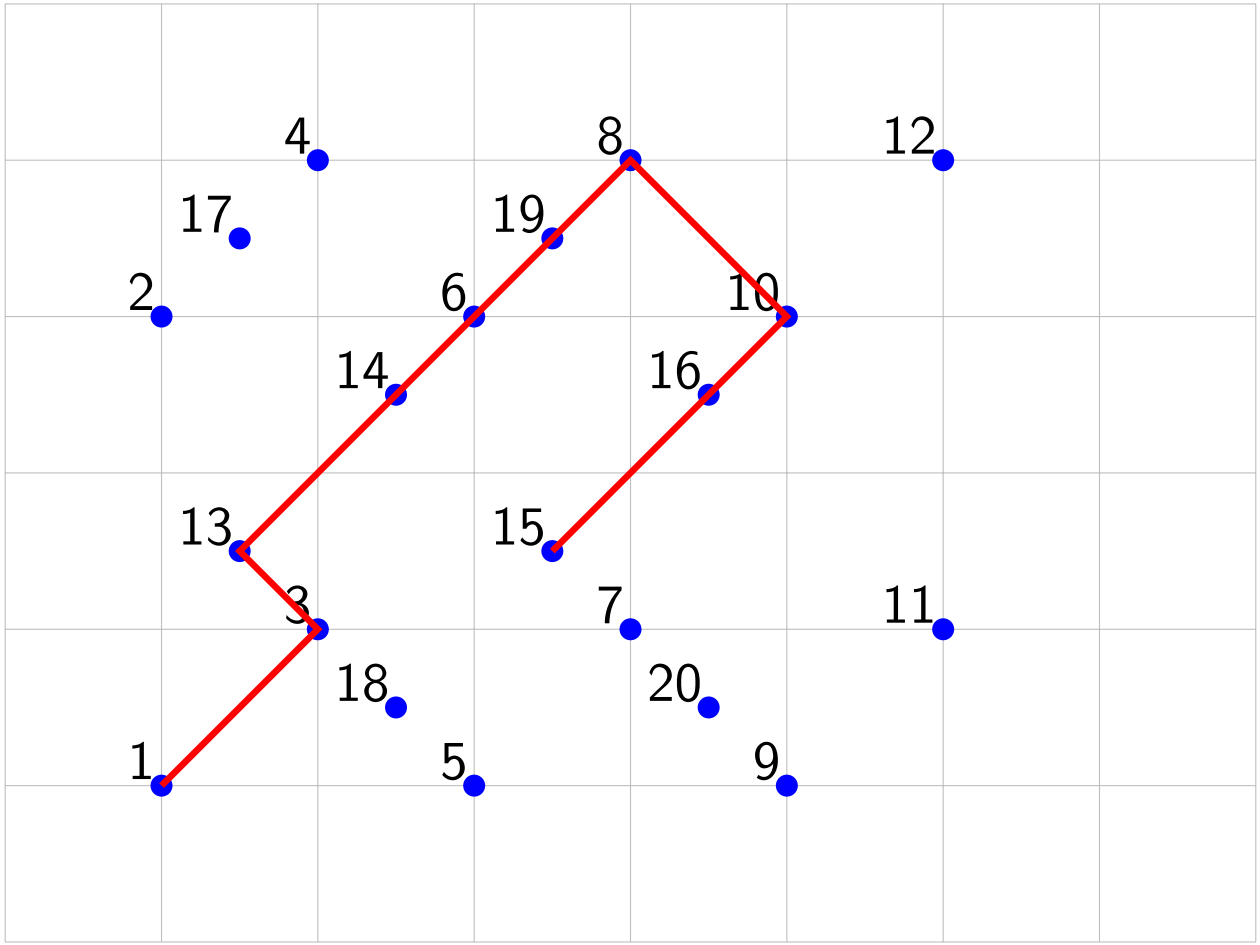
Nearest Neighbor Example



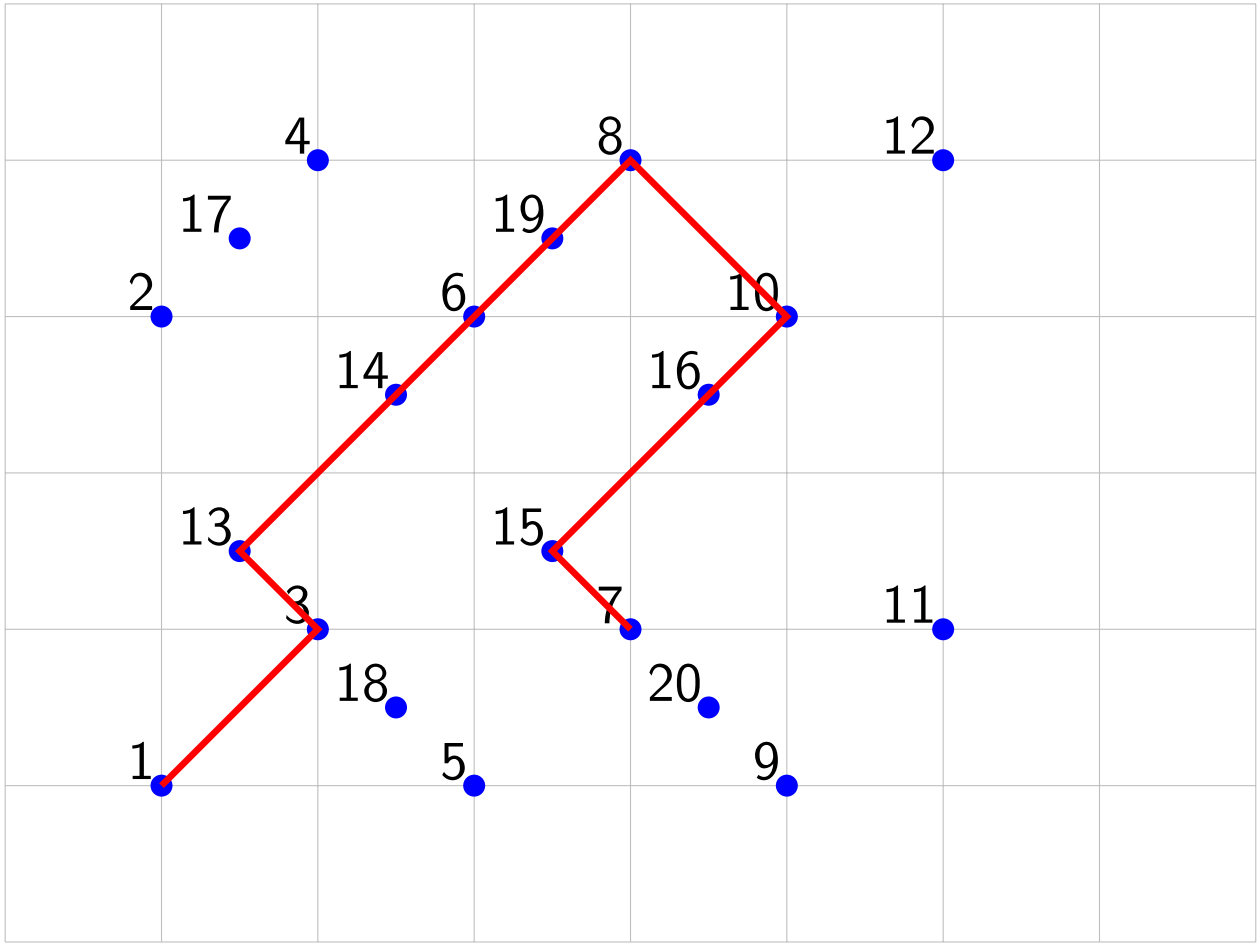
Nearest Neighbor Example



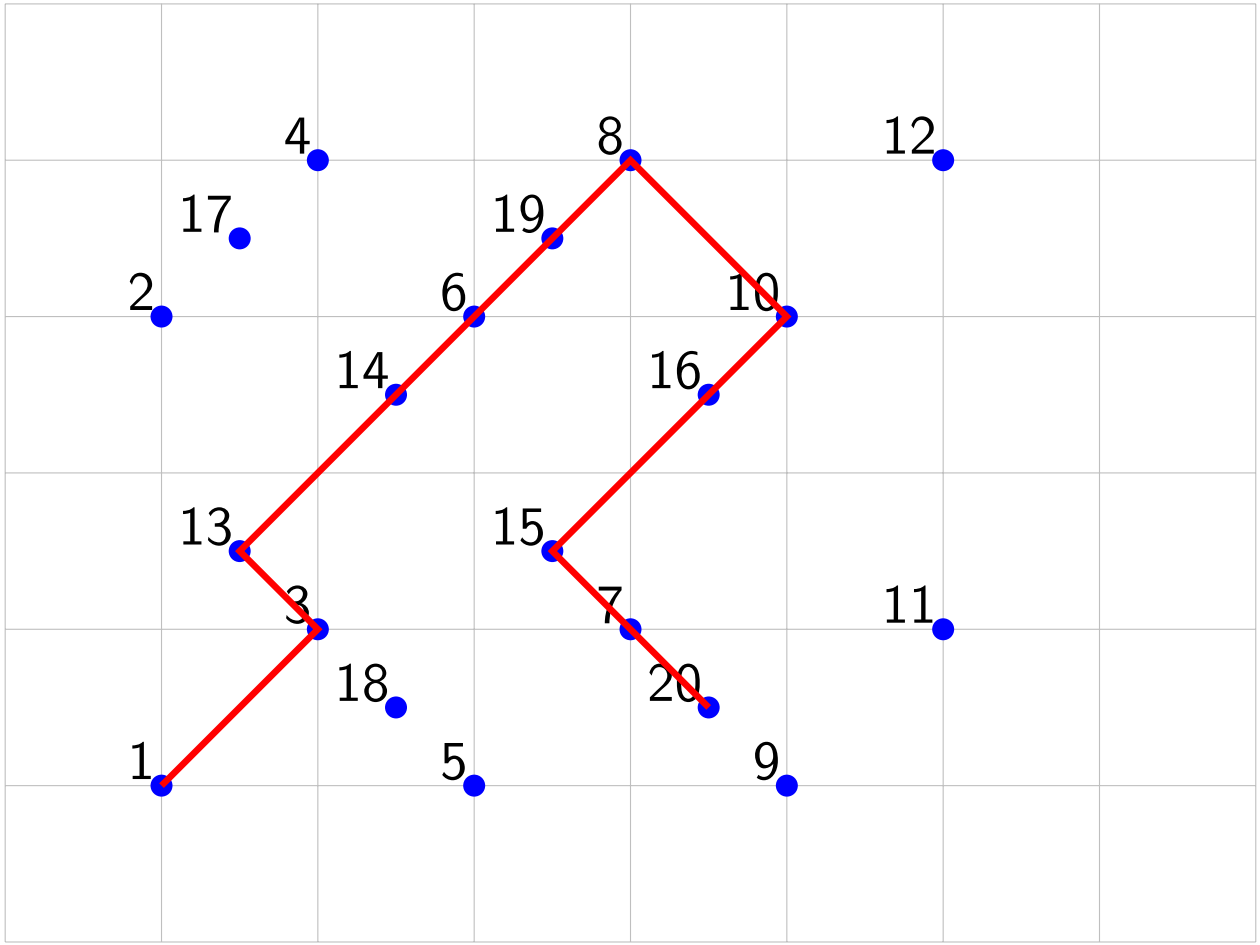
Nearest Neighbor Example



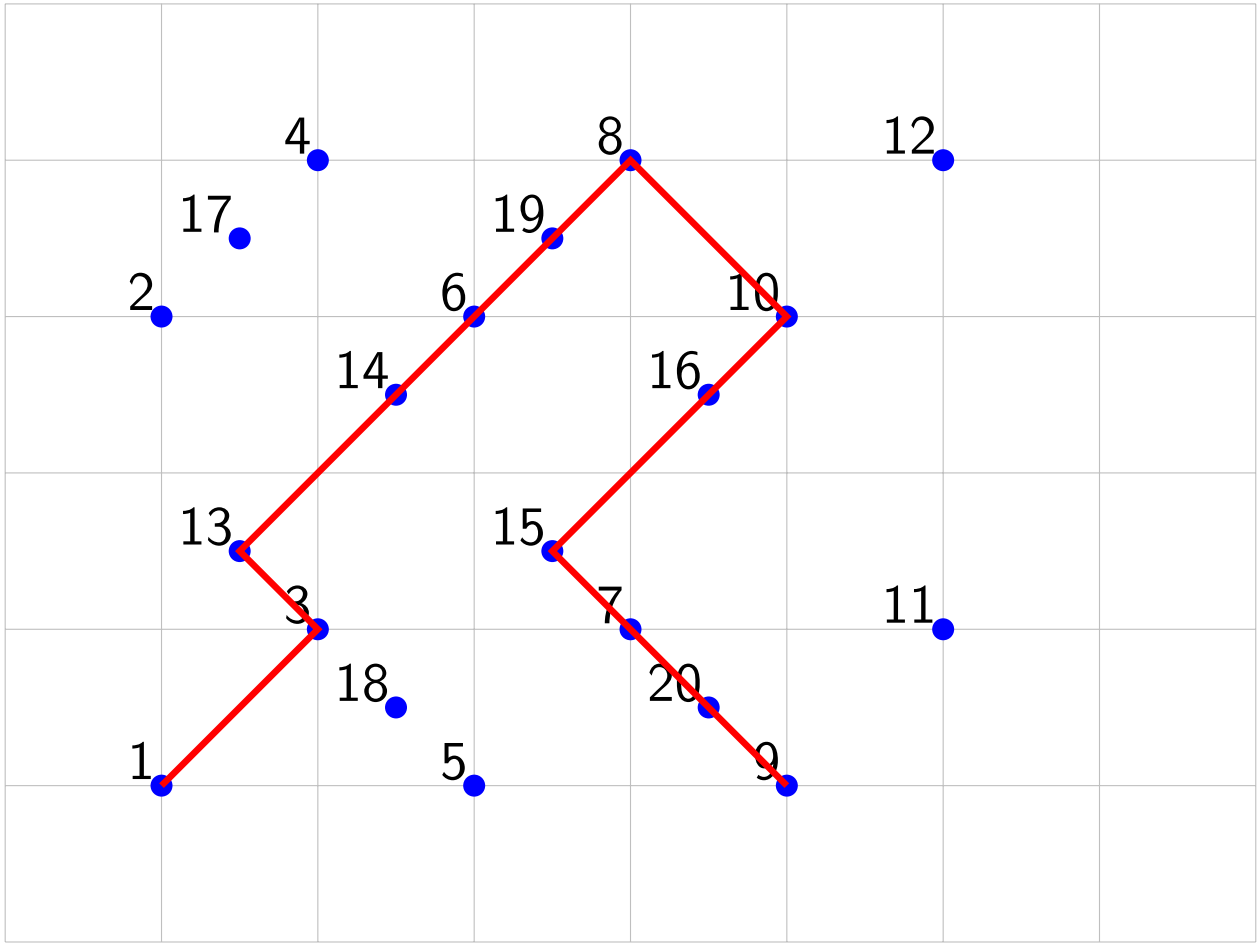
Nearest Neighbor Example



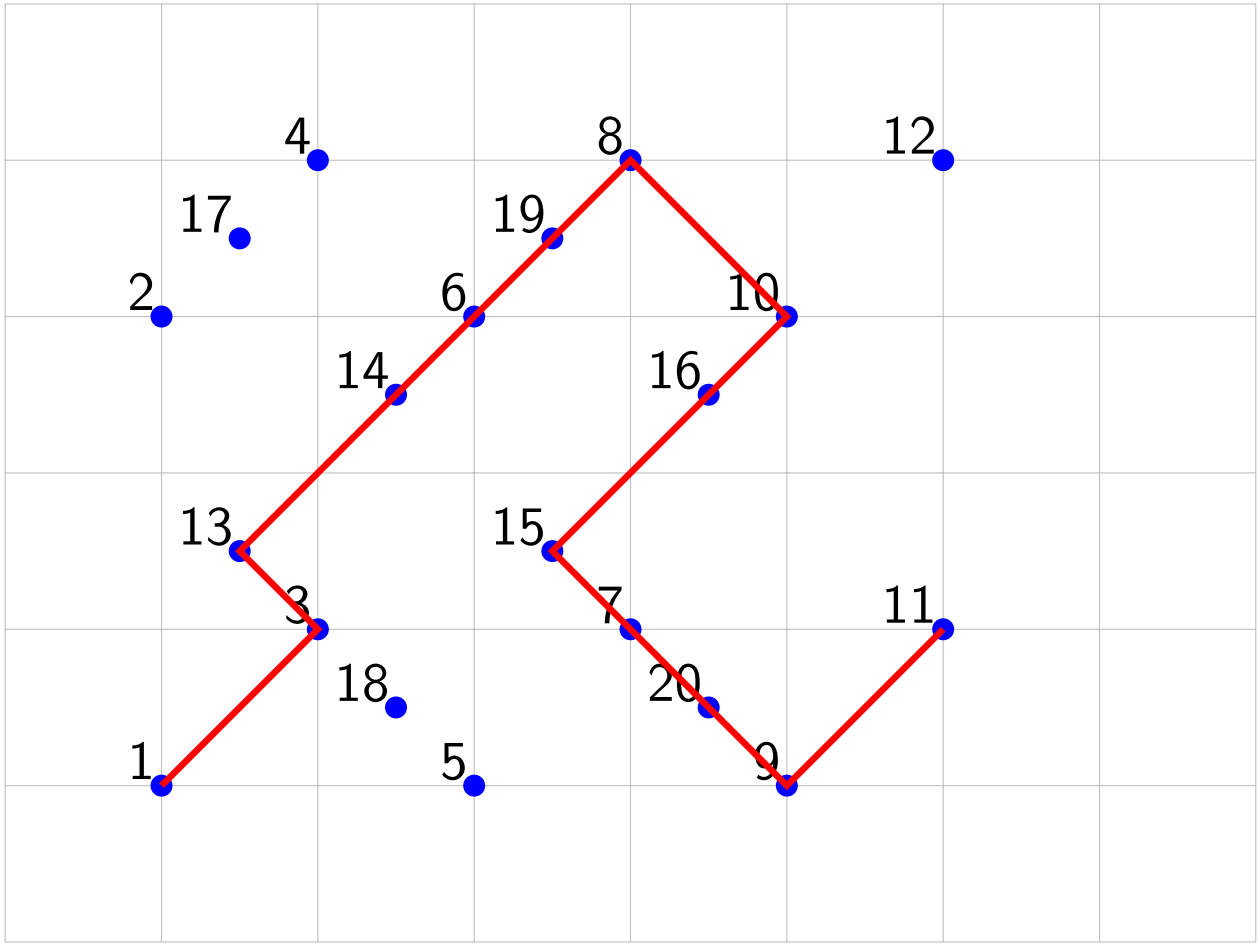
Nearest Neighbor Example



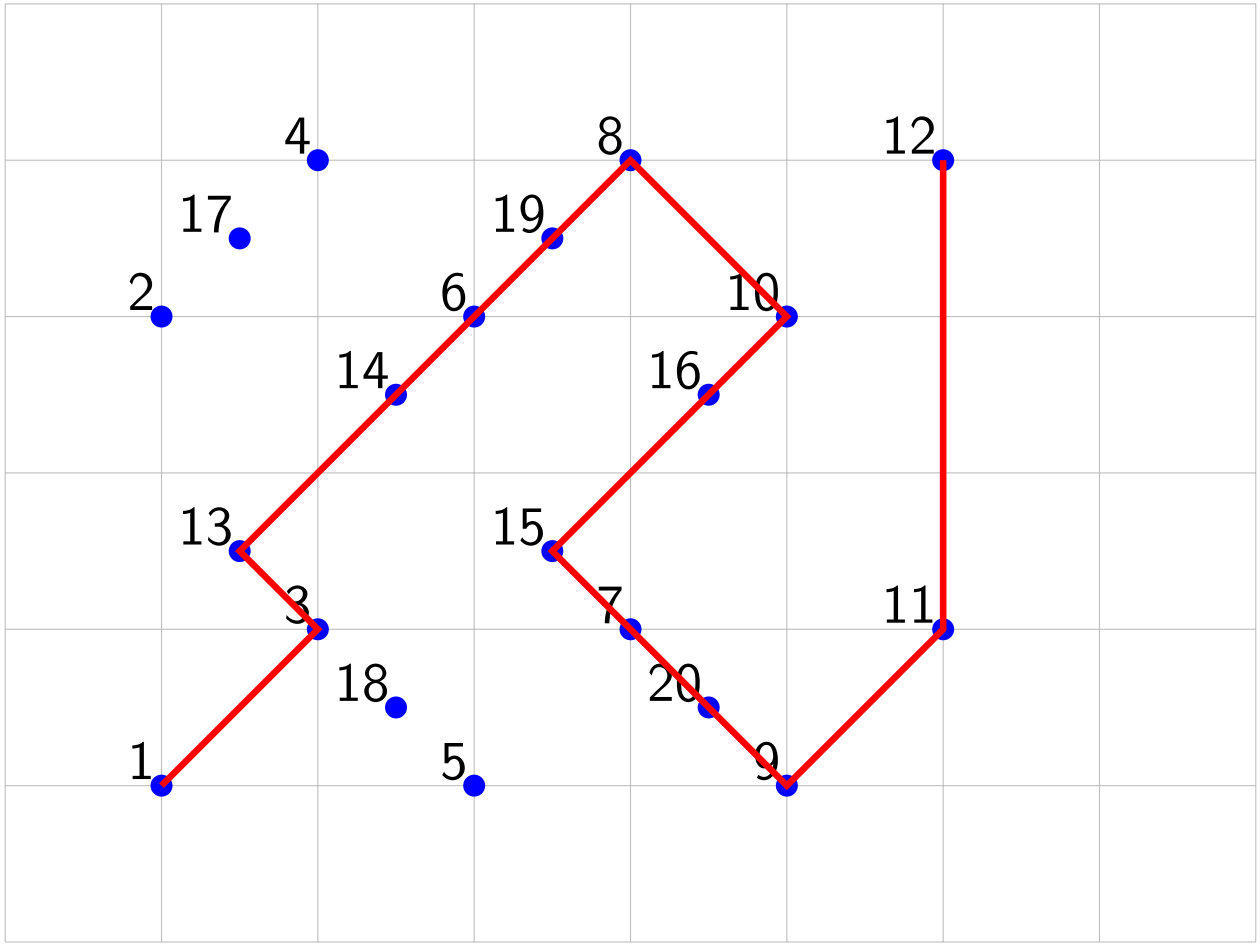
Nearest Neighbor Example



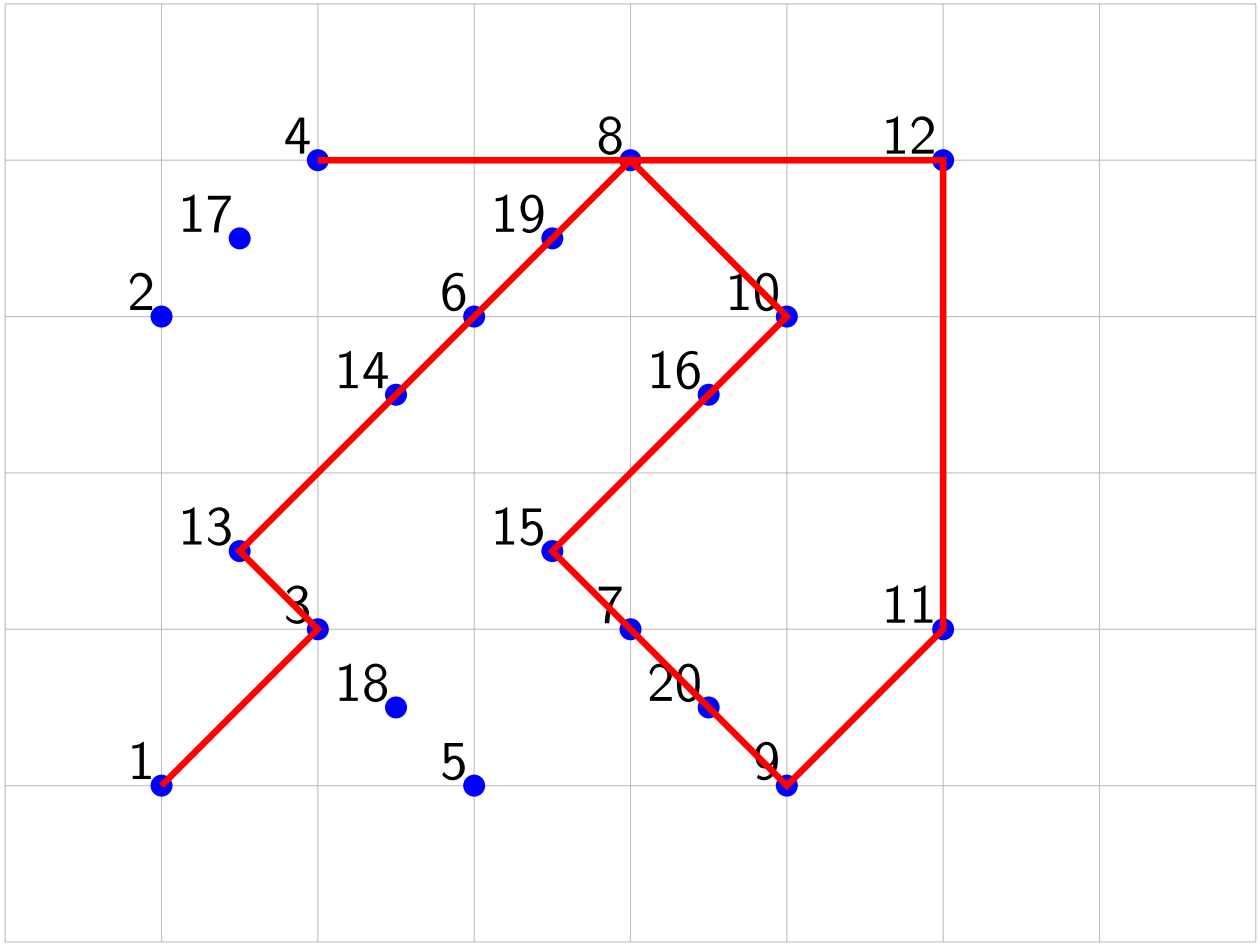
Nearest Neighbor Example



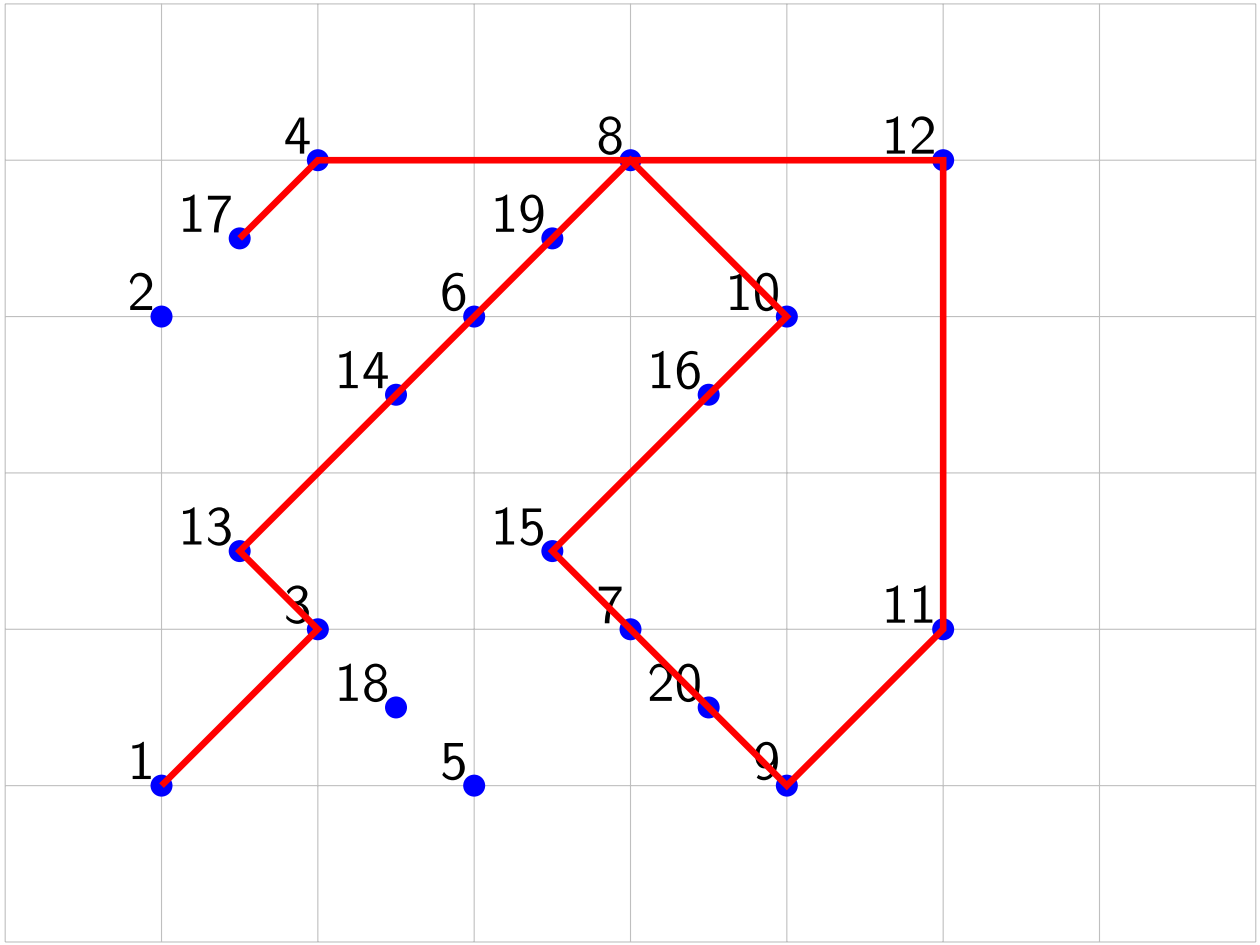
Nearest Neighbor Example



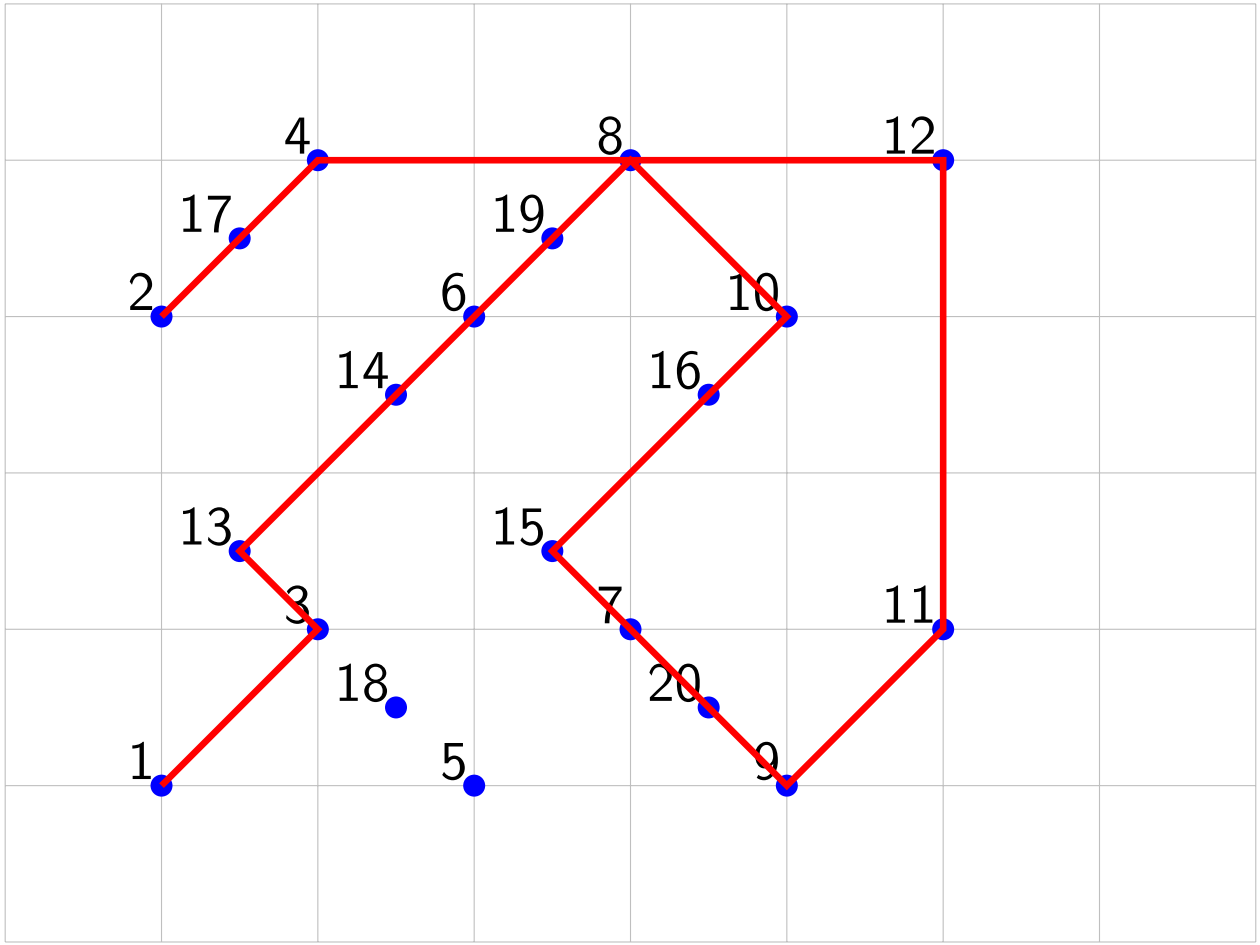
Nearest Neighbor Example



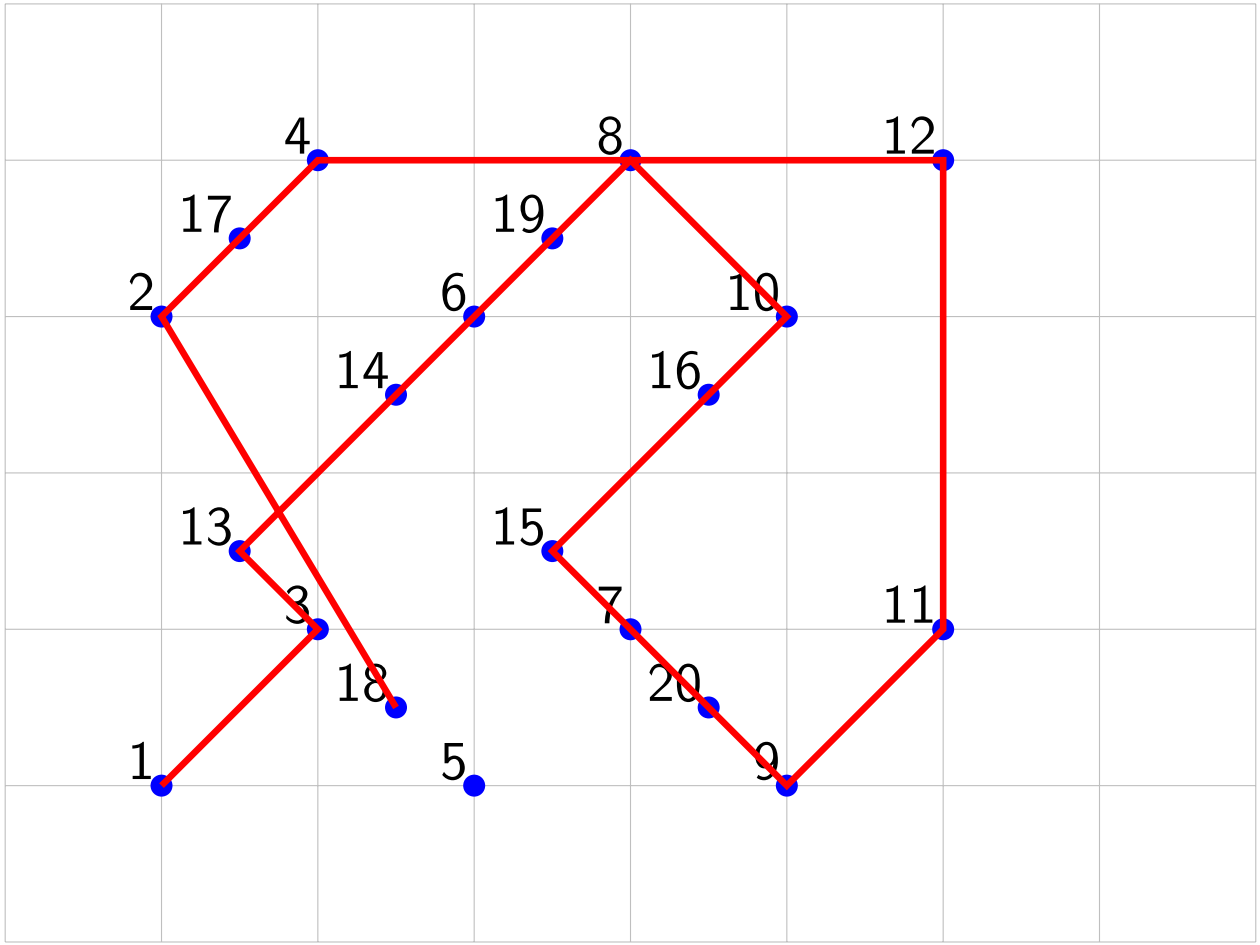
Nearest Neighbor Example



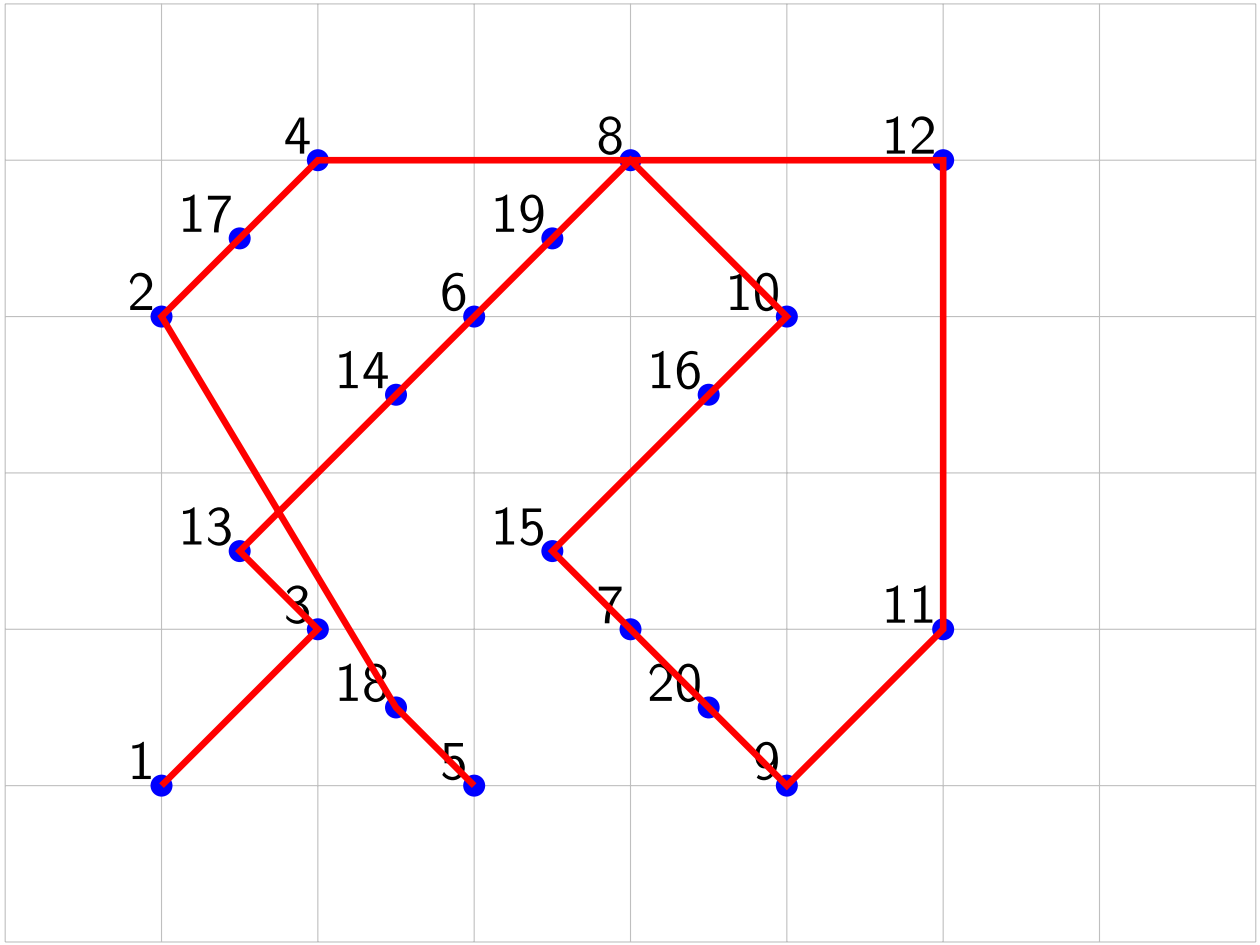
Nearest Neighbor Example



Nearest Neighbor Example

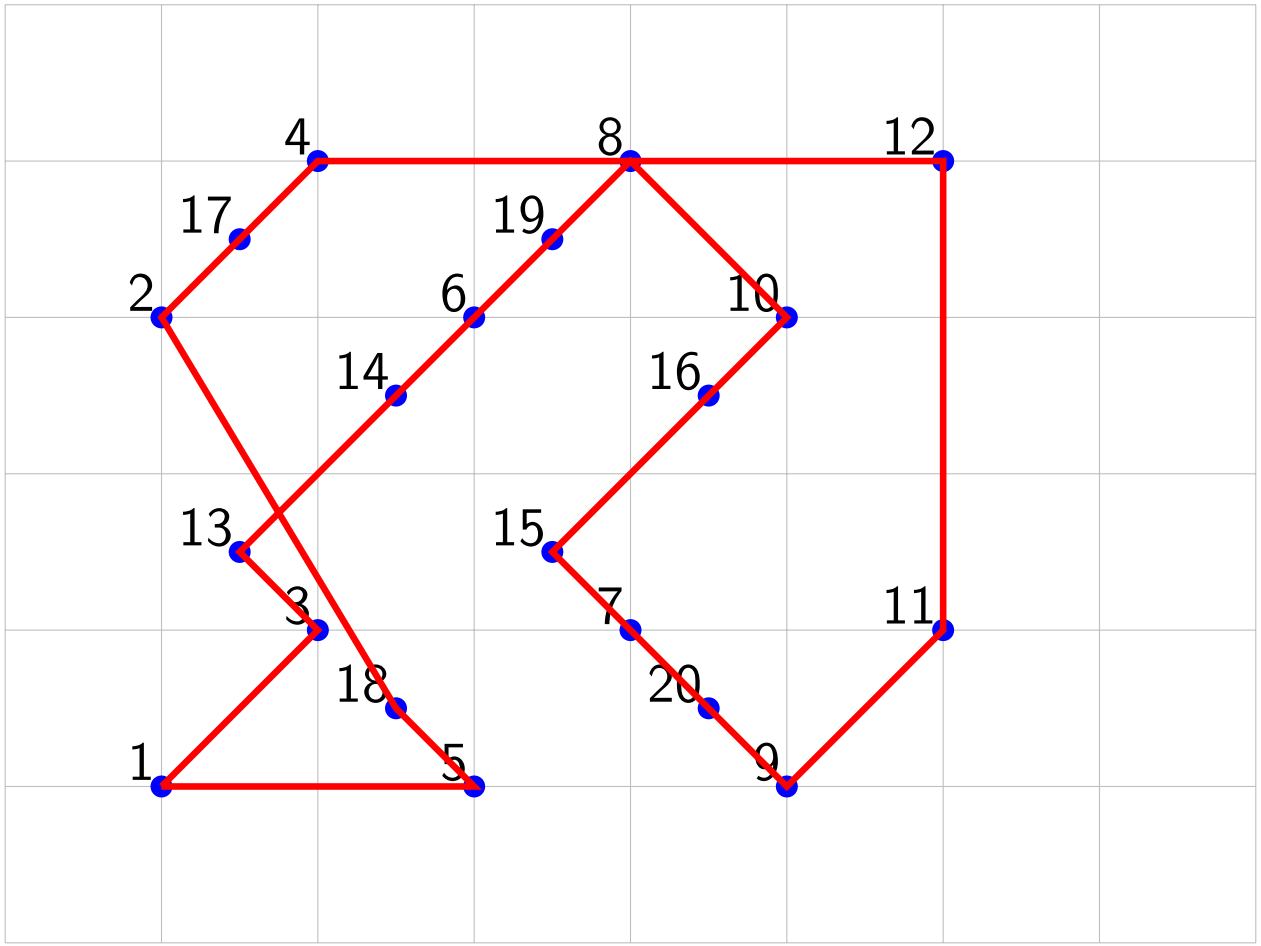


Nearest Neighbor Example



Nearest Neighbor Example

Total cost = 26.765



Sorted Edges Heuristic

Greedy heuristic!

- Sort the edges in nondecreasing order;
- Select the cheapest edge, if feasible, add the edge to the solution;
- Repeat until all cities are connected;
- Return to the starting city to complete the Hamiltonian tour.
- Not the nearest neighbor.

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Sorted Edges Heuristic

Input: N cities with pairwise distances $d_{(i,j)}$
Output: A tour that visits each city exactly once and returns to the starting city

Sort = Sort the edges (i, j) in nondecreasing order of cost $d_{(i,j)}$;
Initialize a list of connected components C;
$C = \{\{i\} : \forall i \in N\}$;
while $|C| > 1$ **do**
  for *edge* (i, j) *in the sorted list* **do**
    if *adding edge* (i, j) *does not violate any constraints* **then**
      Create a new component $c(i - -j)$ that connects $c(i)$ to $c(j)$;
      Add $c(i - -j)$ to the list of components C.;
      Remove components c(i) and c(j) from C;
    end
  end
end
Return to the starting city to complete the tour;

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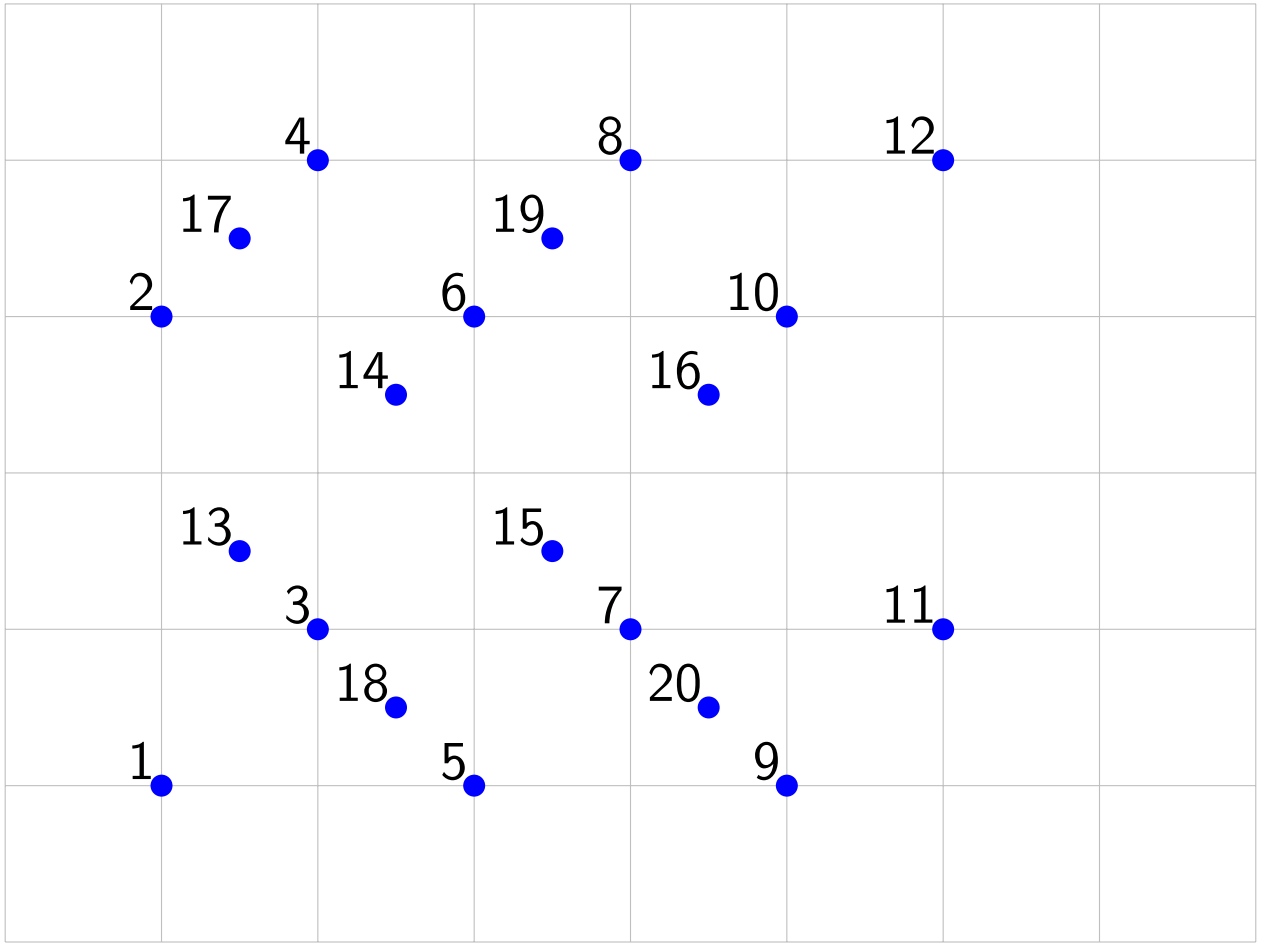
Sorted edges Example



Sorted edges Example

List of sorted edges = {(2, 17), (3, 13), (3, 18), (4, 17), (5, 18), (6, 14), (6, 19), (7, 15), (7, 20), (8, 19), (9, 20), (10, 16), (1, 3), (2, 4), (3, 5), (4, 6), (5, 7), (6, 8), (7, 9), (8, 10), (9, 11), (10, 12), (13, 14), (13, 18), (14, 15), (14, 17), (14, 19), (15, 16), (15, 18), (15, 20), (16, 19), (1, 13), (1, 18), (2, 13), (2, 14), (3, 14), (3, 15), (4, 14), (4, 19), (5, 15), (5, 20), (6, 15), (6, 16), (6, 17), (7, 16), (7, 18), (8, 16), (10, 19), (11, 20), (1, 5), (2, 6), (3, 7), (4, 8), (5, 9), (6, 10), (7, 11), (8, 12), (13, 15), (13, 17), (14, 16), (14, 18), (15, 19), (16, 20), (17, 19), (18, 20), (5, 13), (6, 13), (7, 14), (8, 14), (9, 15), (10, 15), (11, 16), (12, 16), (2, 3), (3, 6), (6, 7), (7, 10), (10, 11), (2, 19), (3, 17), (3, 20), (4, 13), (5, 14), (6, 18), (7, 13), (7, 19), (8, 15), (8, 17), (9, 16), (9, 18), (10, 14), (10, 20), (11, 15), (12, 19), (13, 19), (14, 20), (15, 17), (16, 18), (1, 14), (1, 15), (2, 15), (2, 18), (3, 16), (3, 19), (4, 15), (4, 16), (5, 16), (6, 20), (1, 2), (3, 4), (5, 6), (7, 8), (9, 10), (11, 12), (1, 7), (2, 8), (3, 9), (4, 10), (5, 11), (6, 12), (13, 16), (13, 20), (16, 17), (17, 18), (18, 19), (19, 20), (1, 17), (1, 20), (2, 16), (4, 18), (5, 19), (7, 17), (8, 13), (8, 20), (9, 14), (10, 17), (10, 18), (11, 18), (11, 19), (12, 15), (1, 6), (2, 5), (2, 7), (3, 8), (3, 10), (4, 7), (5, 10), (6, 9), (6, 11), (7, 12), (8, 11), (5, 17), (8, 18), (9, 13), (9, 19), (10, 13), (11, 14), (12, 14), (12, 20), (1, 9), (2, 10), (3, 11), (4, 12), (1, 4), (4, 5), (5, 8), (8, 9), (9, 12), (17, 20), (1, 16), (1, 19), (2, 20), (4, 20), (11, 13), (12, 17), (9, 17), (12, 18), (1, 8), (1, 10), (2, 9), (3, 12), (4, 9), (4, 11), (5, 12), (1, 11), (2, 12), (11, 17), (12, 13), (2, 11), (1, 12)}

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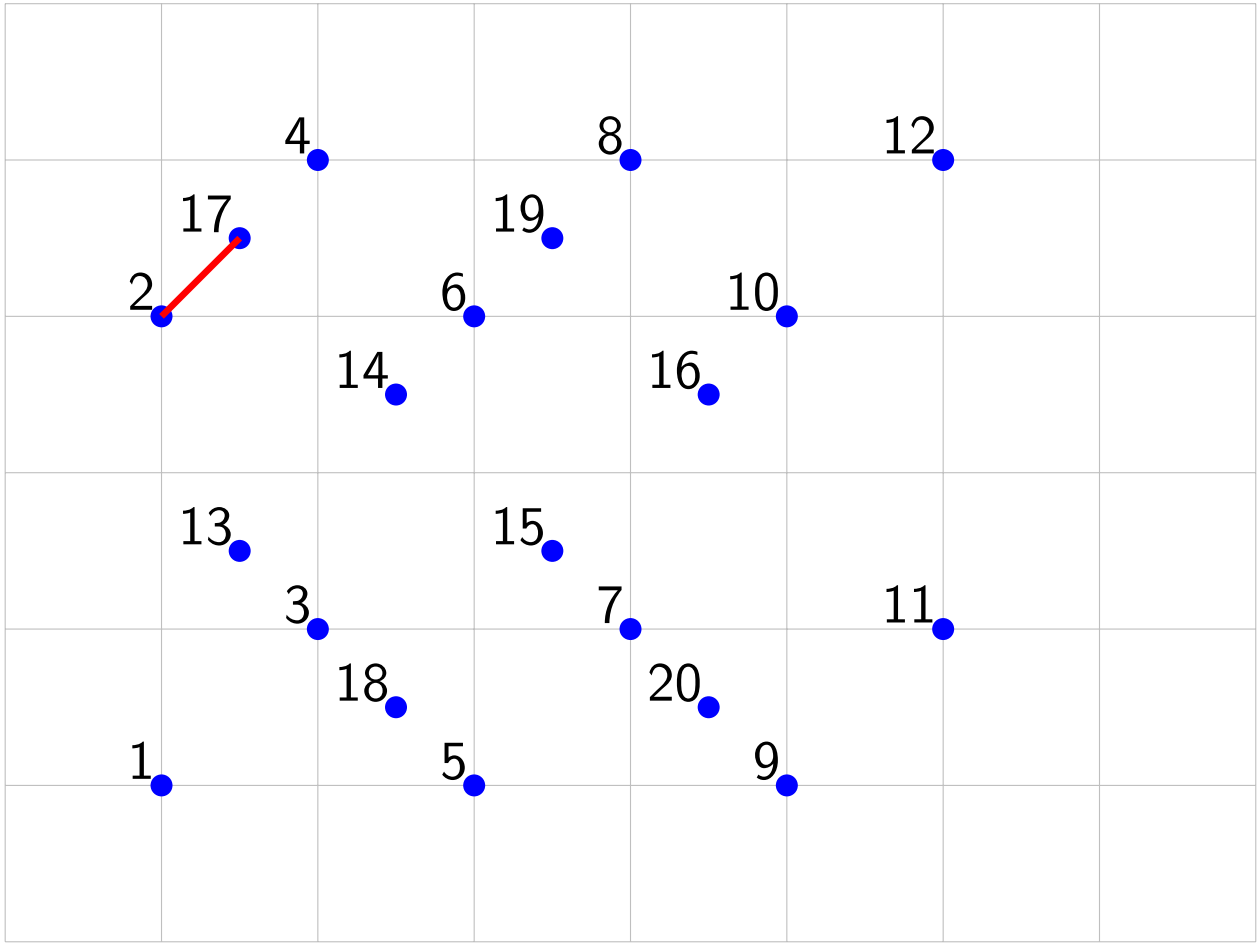
Sorted edges Example

Initialize the set of connected components with a set of singletons for each city.

$$C = \{\{1\},\{2\},\{3\},\{4\},\{5\},\{6\},\{7\},\{8\},\{9\},\{10\},\{11\},\{12\},\{13\},\{14\},\{15\},\{16\},\{17\},\{18\},\{19\},\{20\}\}$$

Sorted edges Example

Next cheapest = (2, 17)



Sorted edges Example

(2, 17)
Add the set $\{2, 17\}$ to C:

$$C = \{\{1\}, \{2\}, \{2, 17\}, \{3\}, \{4\}, \{5\}, \{6\}, \{7\}, \{8\}, \{9\}, \{10\}, \{11\}, \{12\}, \{13\}, \{14\}, \{15\}, \{16\}, \{17\}, \{18\}, \{19\}, \{20\}\}$$

Remove the set $\{2\}$ and $\{17\}$:

$$C = \{\{1\}, \{2, 17\}, \{3\}, \{4\}, \{5\}, \{6\}, \{7\}, \{8\}, \{9\}, \{10\}, \{11\}, \{12\}, \{13\}, \{14\}, \{15\}, \{16\}, \{18\}, \{19\}, \{20\}\}$$

$$|C| = 19$$

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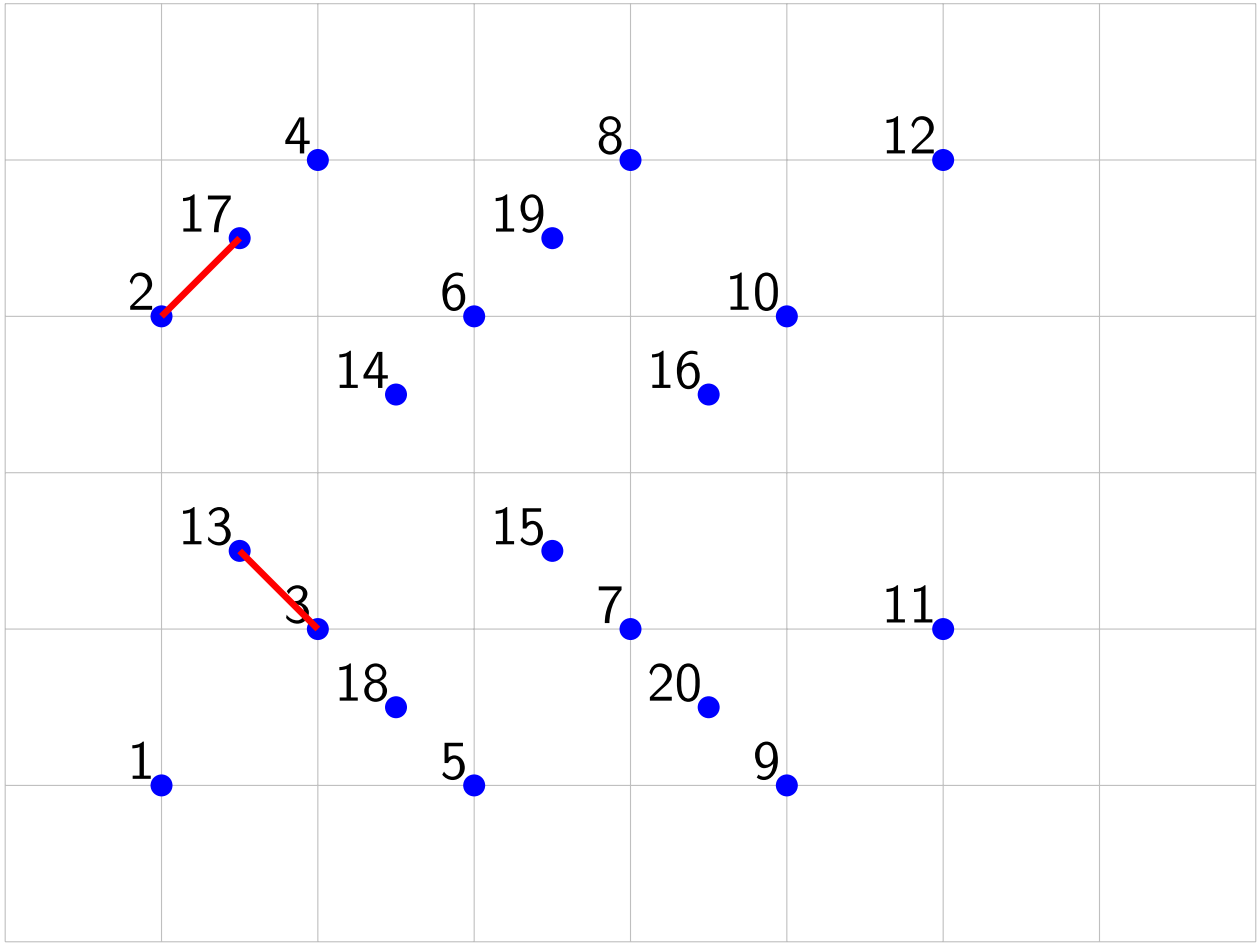
Sorted edges Example

Next cheapest = (3, 13)



Sorted edges Example

(3, 13)
Add the set $\{3, 13\}$ to C:

$$C = \{\{1\}, \{2, 17\}, \{3, 13\}, \{3\}, \{4\}, \{5\}, \{6\}, \{7\}, \{8\}, \{9\}, \{10\}, \{11\}, \{12\}, \{13\}, \{14\}, \{15\}, \{16\}, \{18\}, \{19\}, \{20\}\}$$

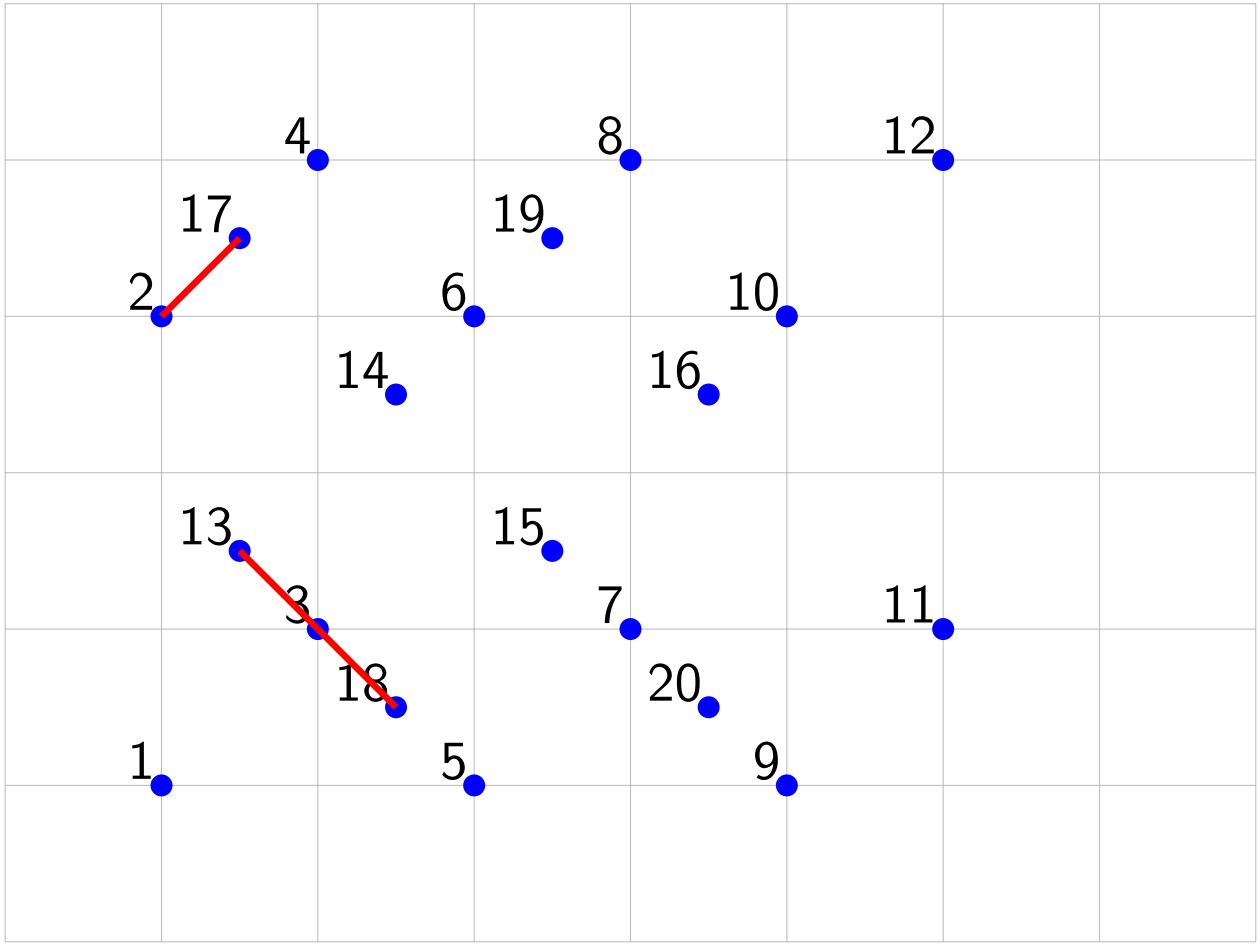
Remove the set $\{3\}$ and $\{13\}$:

$$C = \{\{1\}, \{2, 17\}, \{3, 13\}, \{4\}, \{5\}, \{6\}, \{7\}, \{8\}, \{9\}, \{10\}, \{11\}, \{12\}, \{14\}, \{15\}, \{16\}, \{18\}, \{19\}, \{20\}\}$$

$$|C| = 18$$

Sorted edges Example

Next cheapest = (3, 18)



Sorted edges Example

(3, 18)
Add the set $\{18, 3, 13\}$ to C:

$$C = \{\{1\}, \{2, 17\}, \{18, 3, 13\}, \{3, 13\}, \{4\}, \{5\}, \{6\}, \{7\}, \{8\}, \{9\}, \{10\}, \{11\}, \{12\}, \{14\}, \{15\}, \{16\}, \{18\}, \{19\}, \{20\}\}$$

Remove the set $\{3, 13\}$ and $\{18\}$:

$$C = \{\{1\}, \{2, 17\}, \{18, 3, 13\}, \{4\}, \{5\}, \{6\}, \{7\}, \{8\}, \{9\}, \{10\}, \{11\}, \{12\}, \{14\}, \{15\}, \{16\}, \{19\}, \{20\}\}$$

$$|C| = 17$$

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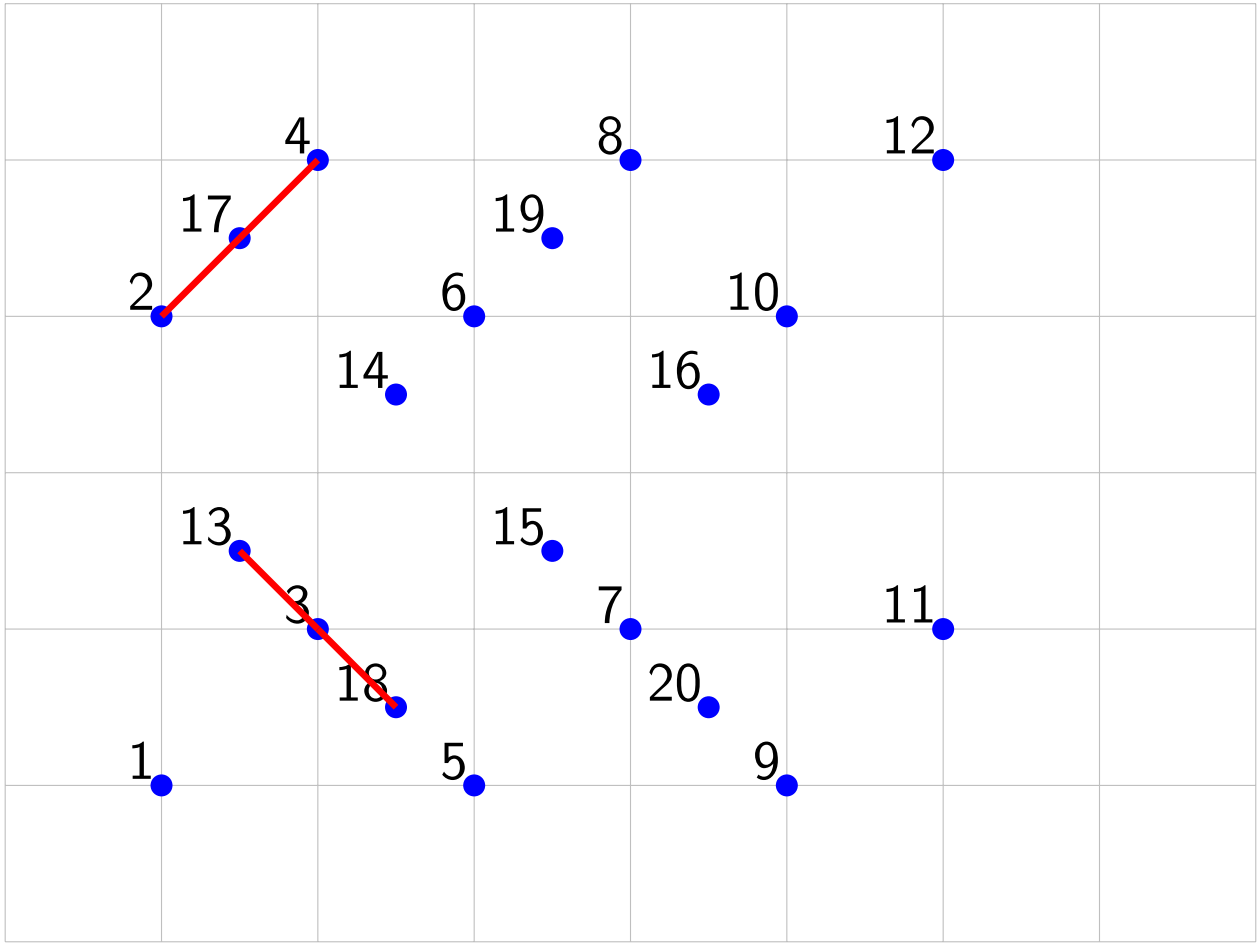
Sorted edges Example

Next cheapest = (4, 17)



Sorted edges Example

(4, 17)
Add the set $\{2, 17, 4\}$ to C:

$$C = \{\{1\}, \{2, 17, 4\}, \{2, 17\}, \{18, 3, 13\}, \{3, 13\}, \{4\}, \{5\}, \{6\}, \{7\}, \{8\}, \{9\}, \{10\}, \{11\}, \{12\}, \{14\}, \{15\}, \{16\}, \{18\}, \{19\}, \{20\}\}$$

Remove the set $\{2, 17\}$ and $\{4\}$:

$$C = \{\{1\}, \{2, 17, 4\}, \{18, 3, 13\}, \{5\}, \{6\}, \{7\}, \{8\}, \{9\}, \{10\}, \{11\}, \{12\}, \{14\}, \{15\}, \{16\}, \{19\}, \{20\}\}$$

$$|C| = 16$$

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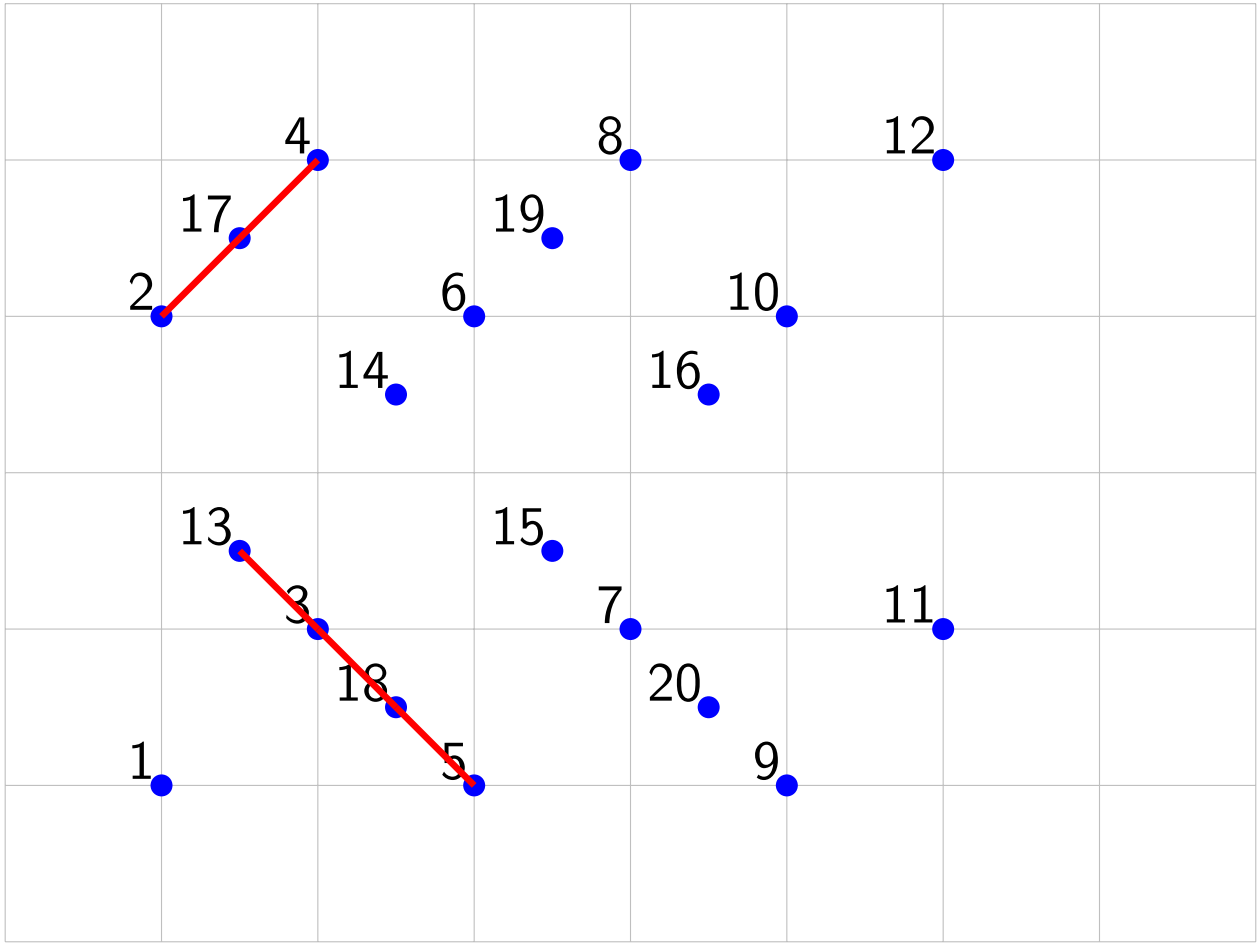
Sorted edges Example

Next cheapest = (5, 18)



Sorted edges Example

(5, 18)
Add the set $\{5, 18, 3, 13\}$ to C:

$$C = \{\{1\}, \{2, 17, 4\}, \{5, 18, 3, 13\}, \{18, 3, 13\}, \{5\}, \{6\}, \{7\}, \{8\}, \{9\}, \{10\}, \{11\}, \{12\}, \{14\}, \{15\}, \{16\}, \{19\}, \{20\}\}$$

Remove the set $\{2, 17\}$ and $\{4\}$:

$$C = \{\{1\}, \{2, 17, 4\}, \{5, 18, 3, 13\}, \{6\}, \{7\}, \{8\}, \{9\}, \{10\}, \{11\}, \{12\}, \{14\}, \{15\}, \{16\}, \{19\}, \{20\}\}$$

$$|C| = 15$$

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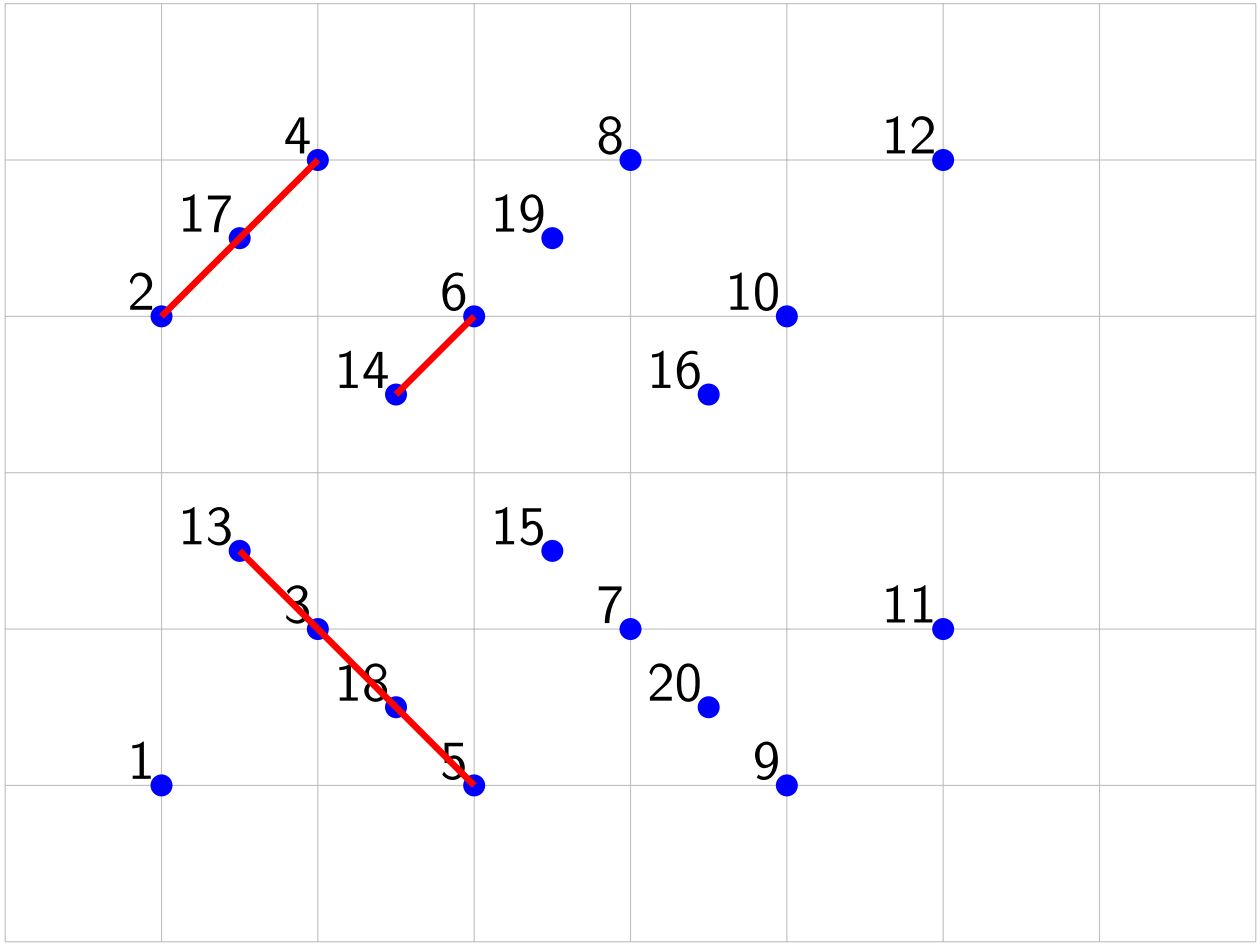
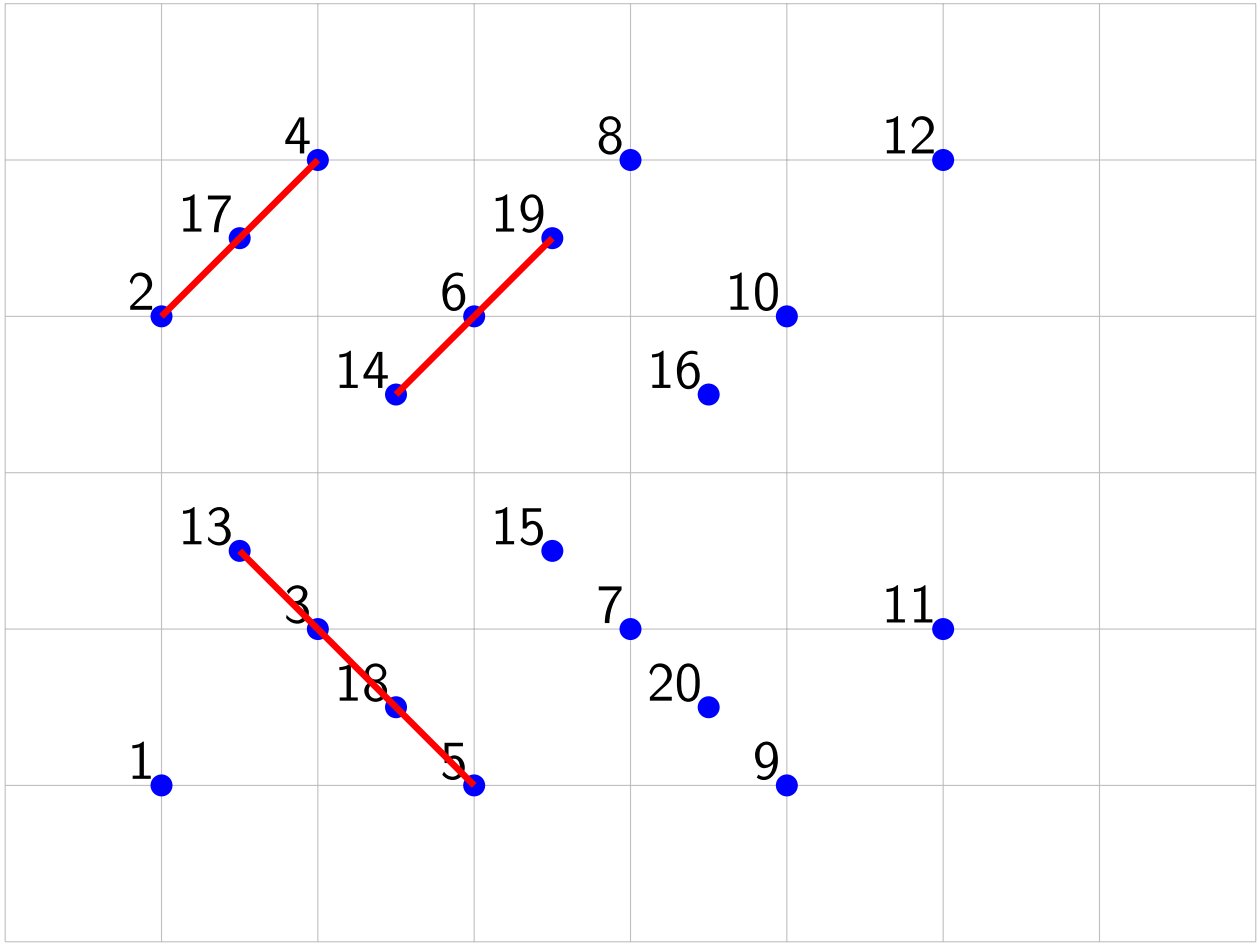
Sorted edges Example

Next cheapest = (6, 14)



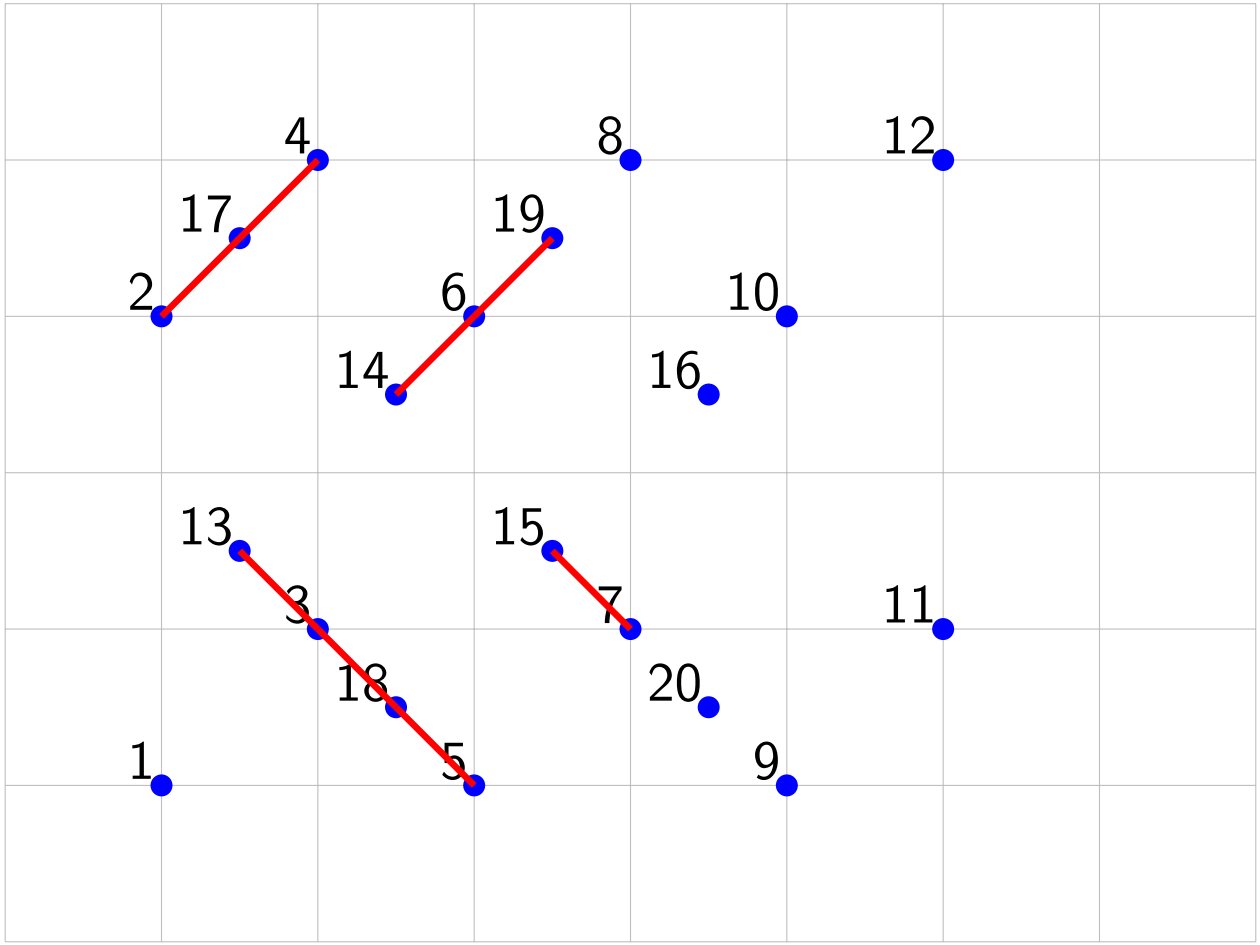
Sorted edges Example

Next cheapest = (6, 19)



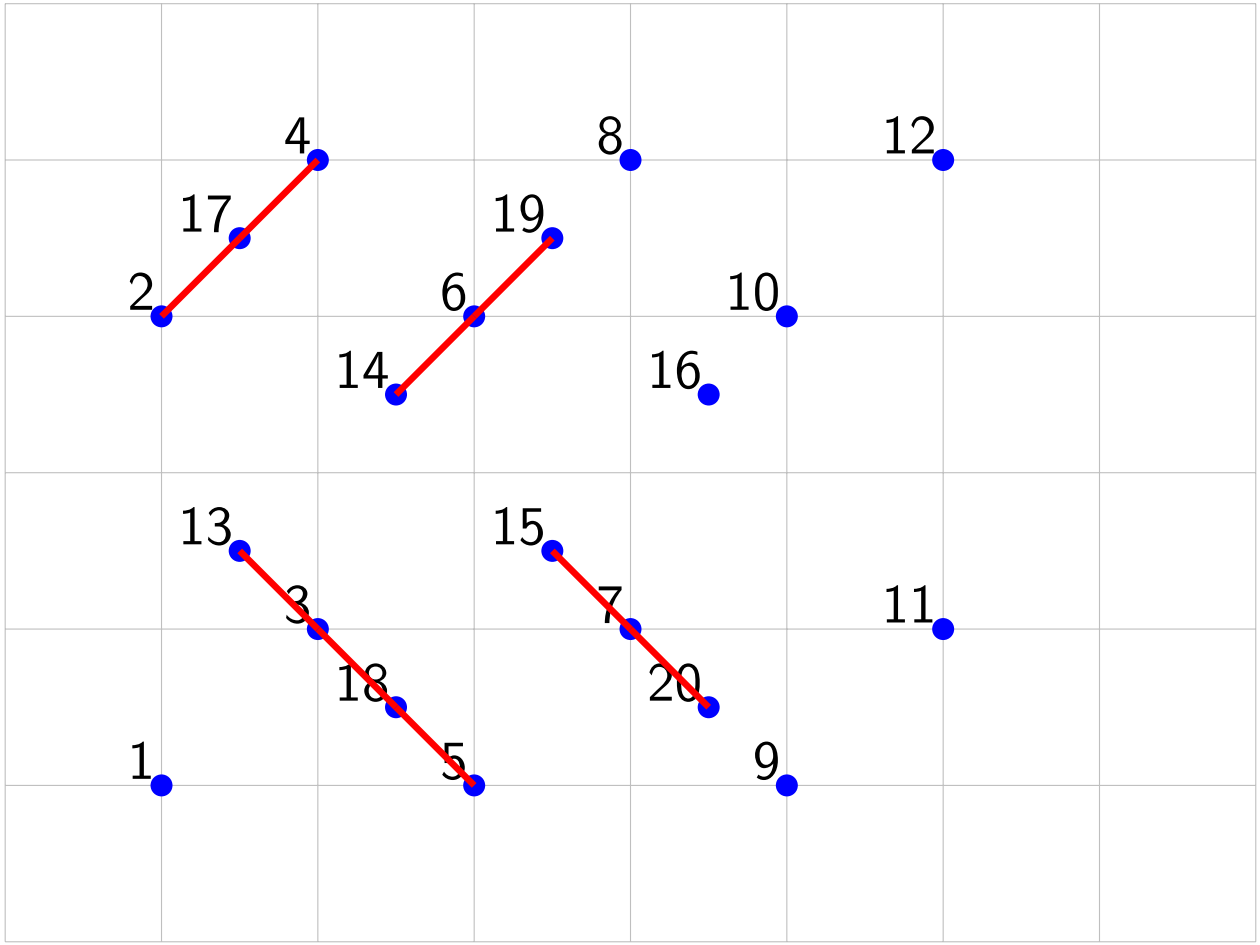
Sorted edges Example

Next cheapest = (7, 15)



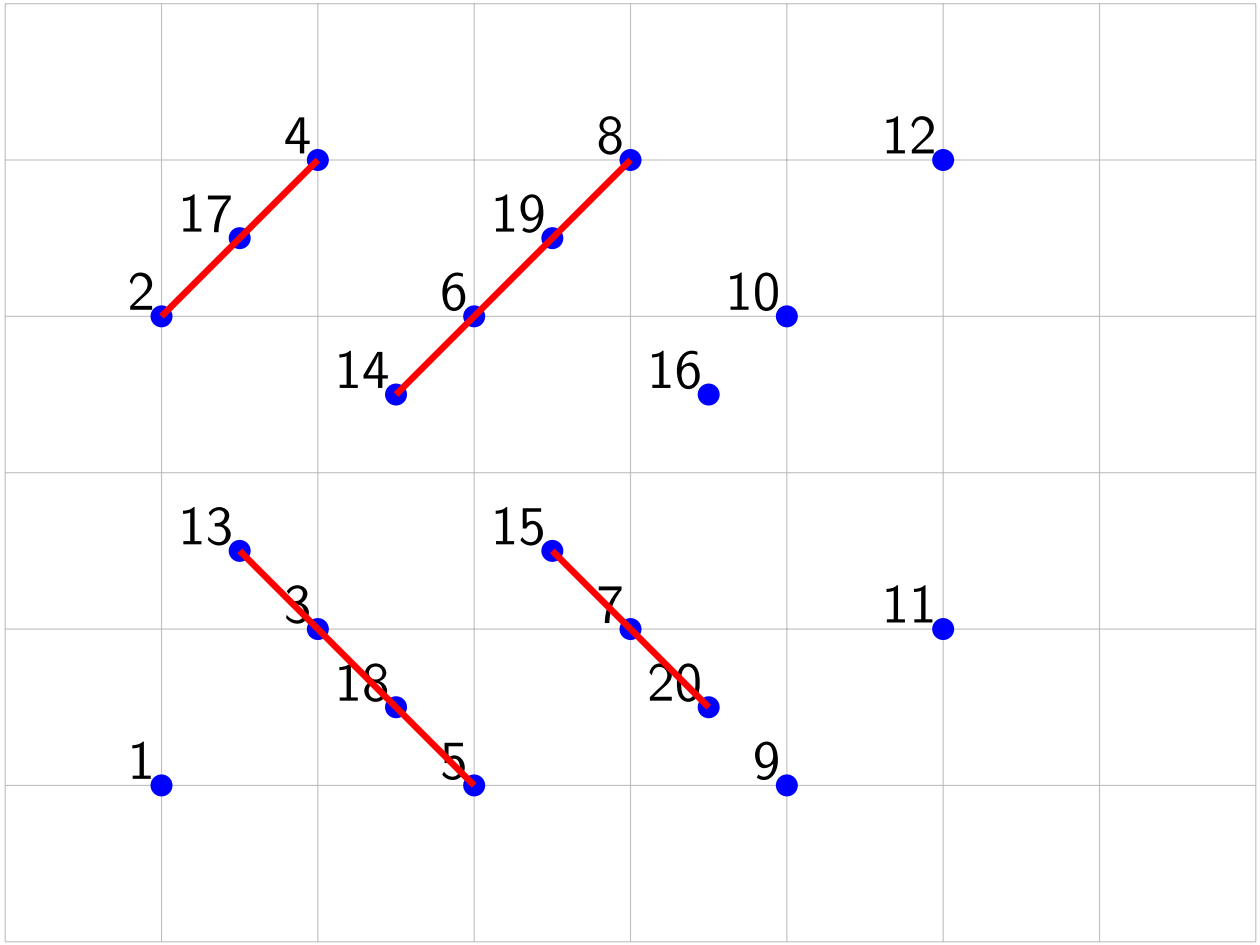
Sorted edges Example

Next cheapest = (7, 20)



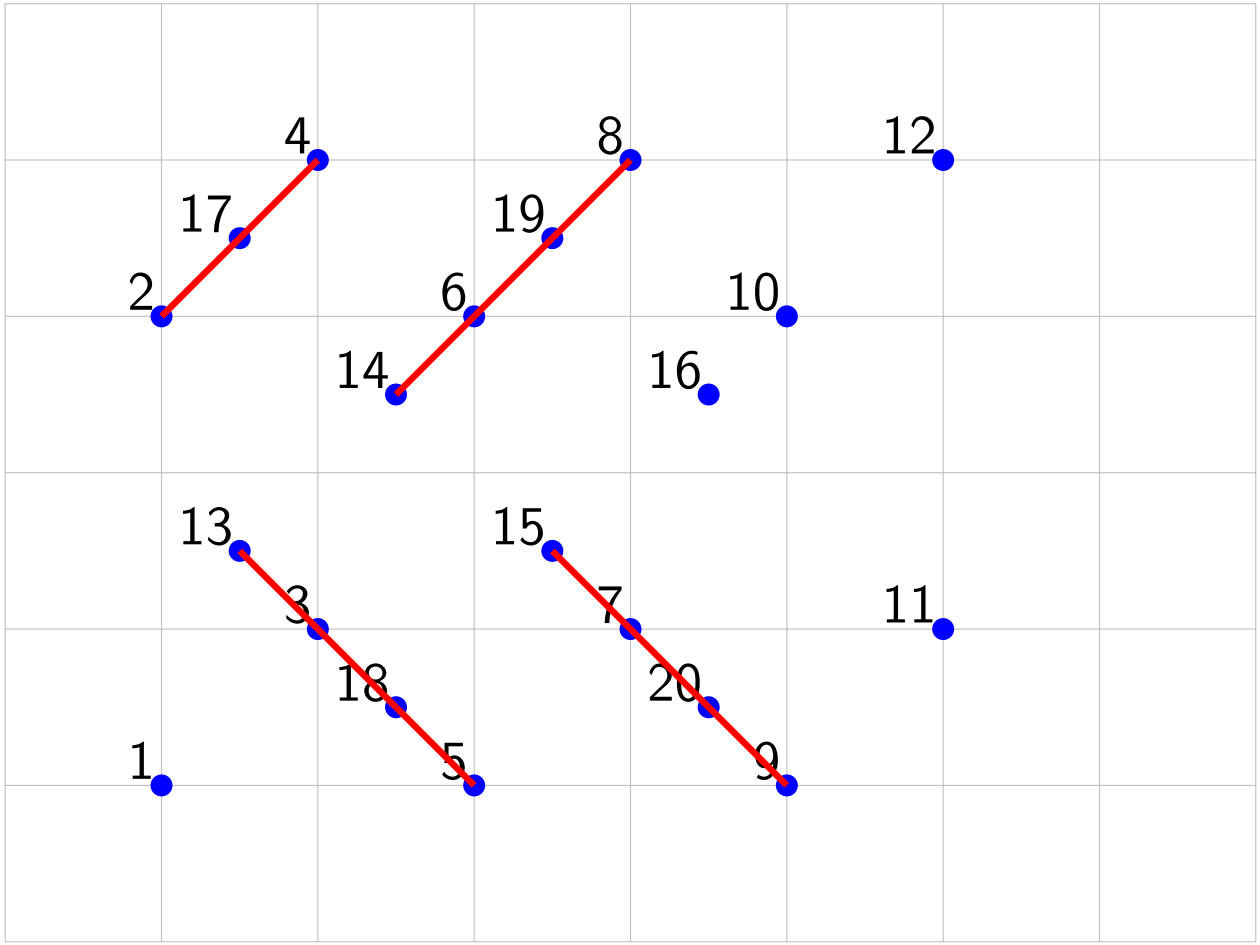
Sorted edges Example

Next cheapest = (8, 19)



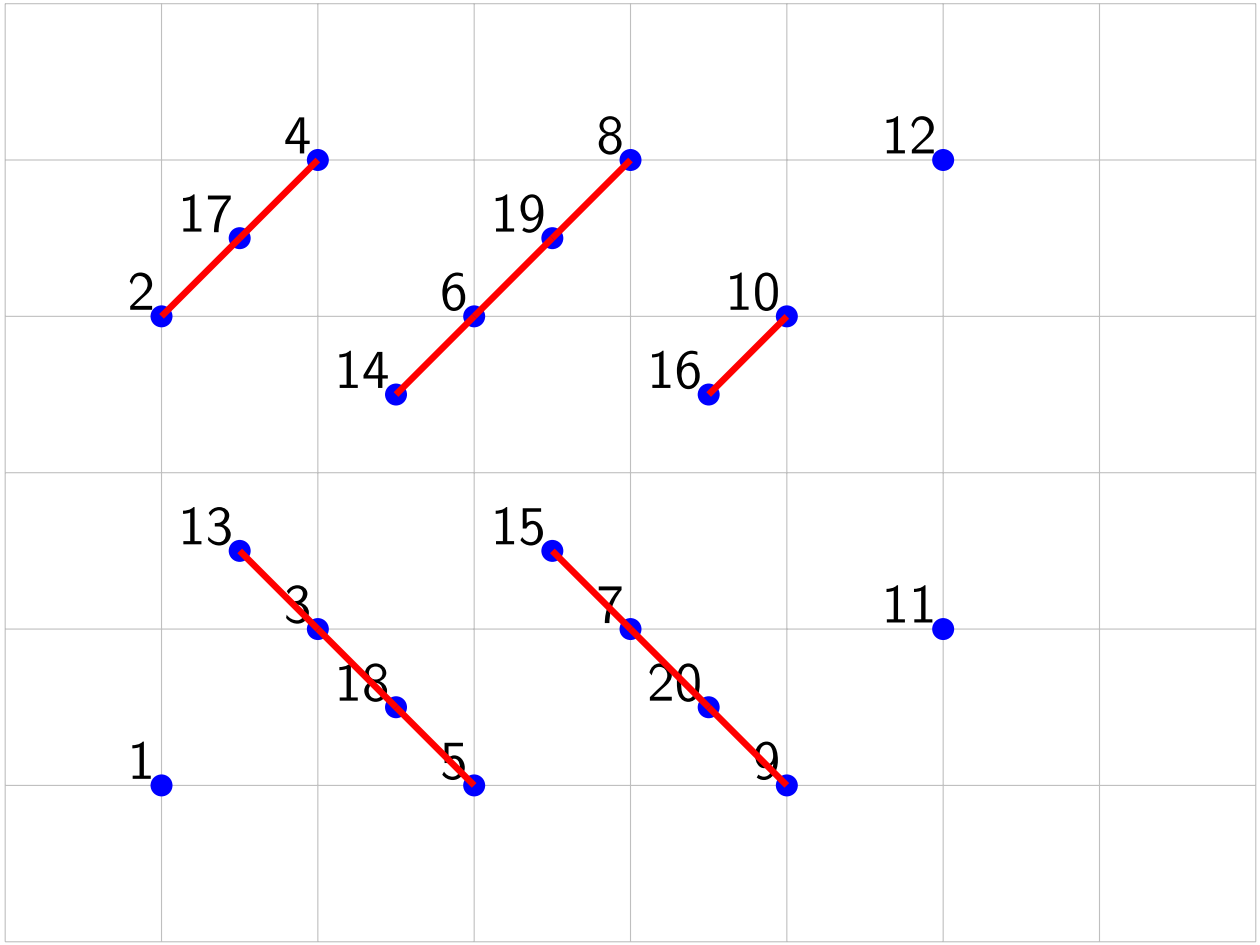
Sorted edges Example

Next cheapest = (9, 20)



Sorted edges Example

Next cheapest = (10, 16)



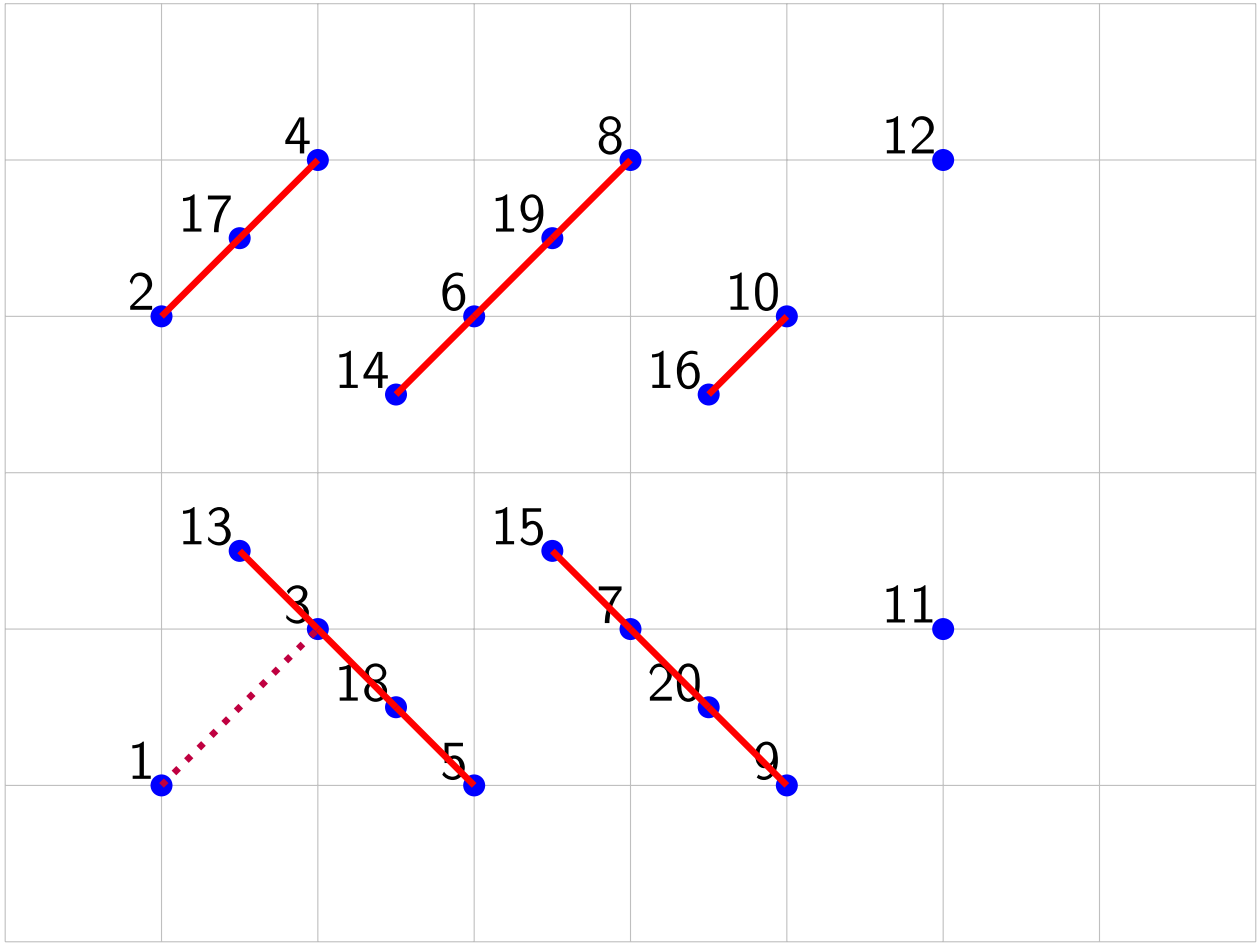
Sorted edges Example

$$C = \{\{1\}, \{2, 17, 4\}, \{5, 18, 3, 13\}, \{14, 6, 19, 8\}, \{9, 20, 7, 15\}, \{10, 16\}, \{11\}, \{12\}\}$$

$$|C| = 8$$

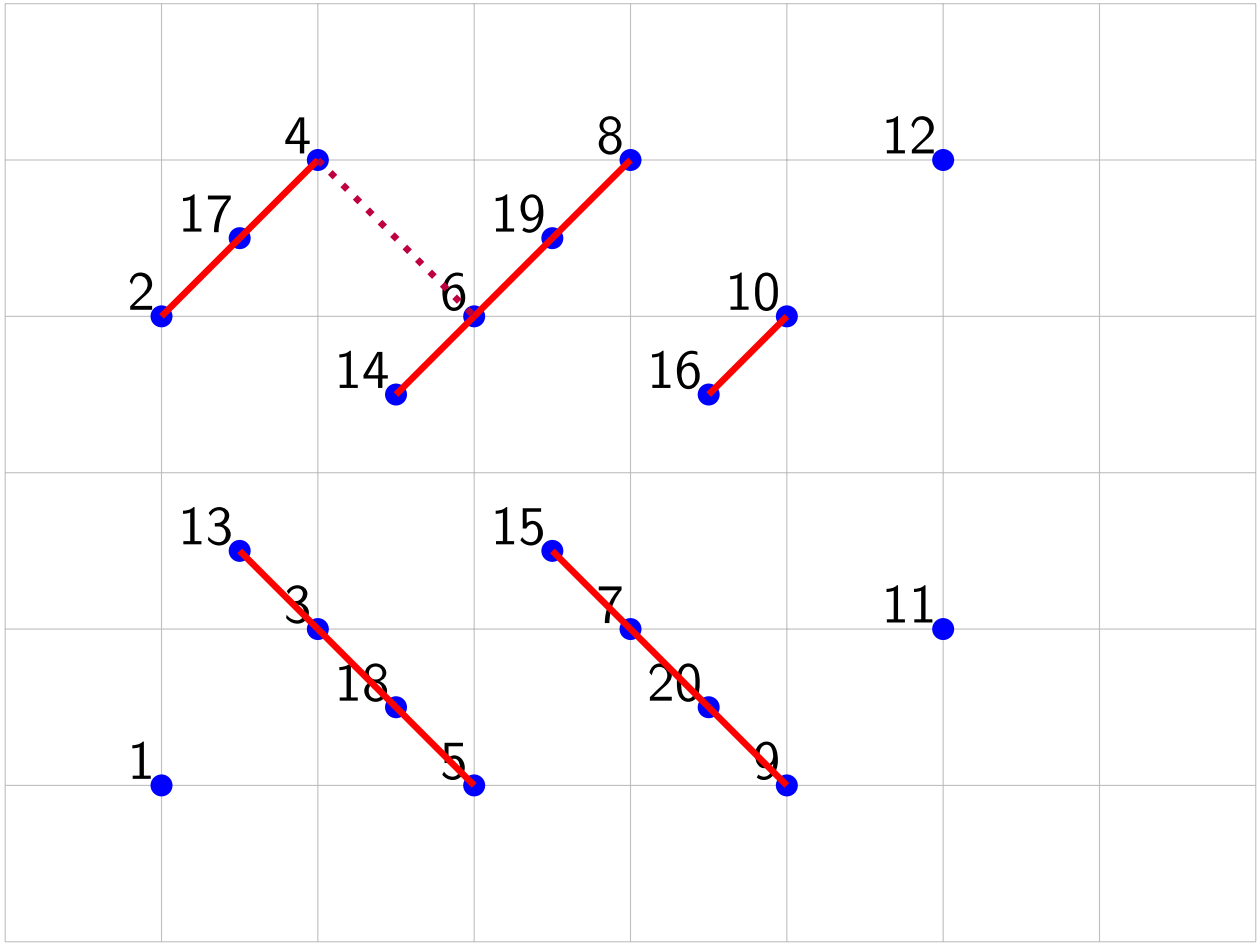
Sorted edges Example

Next cheapest = (1, 3)



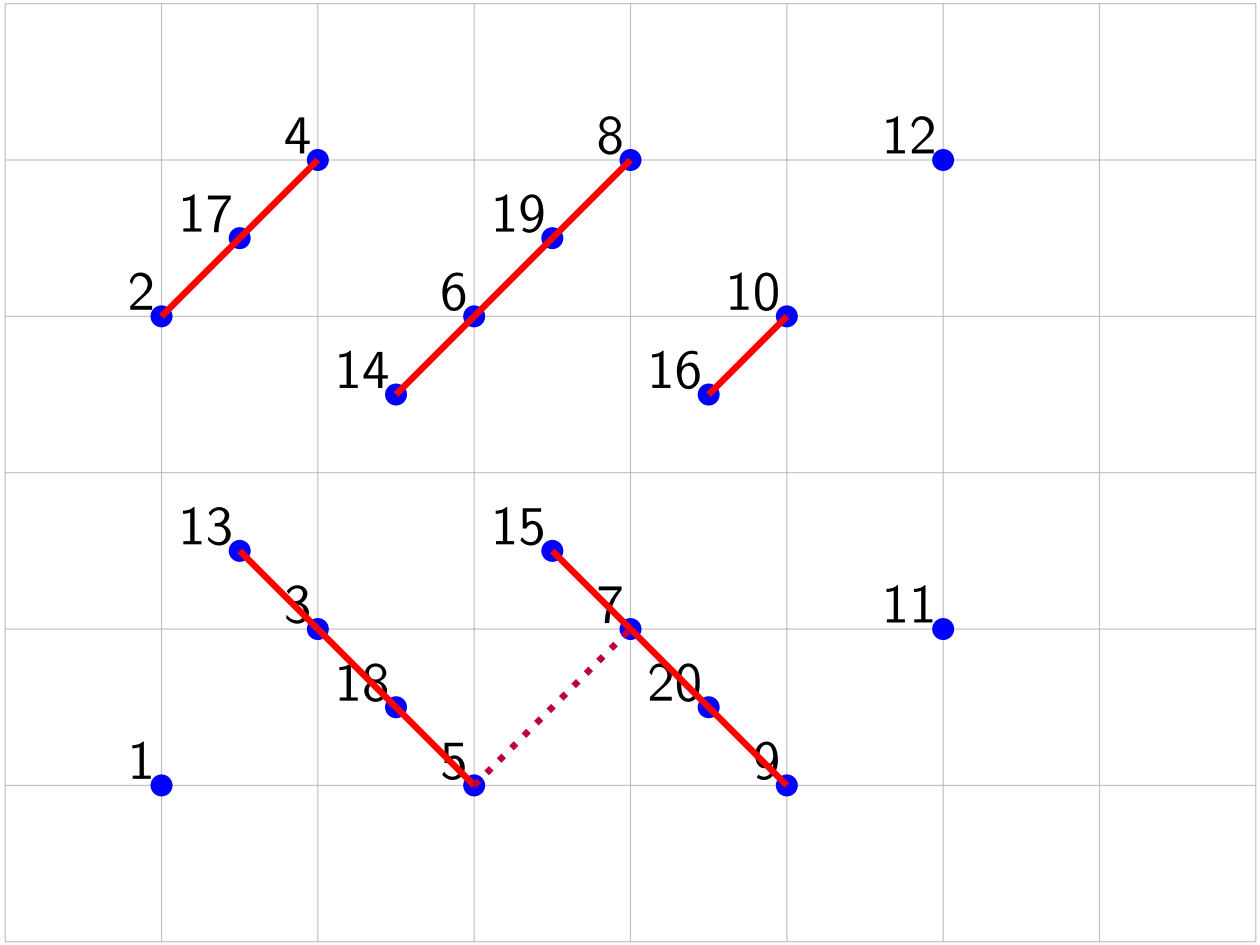
Sorted edges Example

Next cheapest = (4, 6)



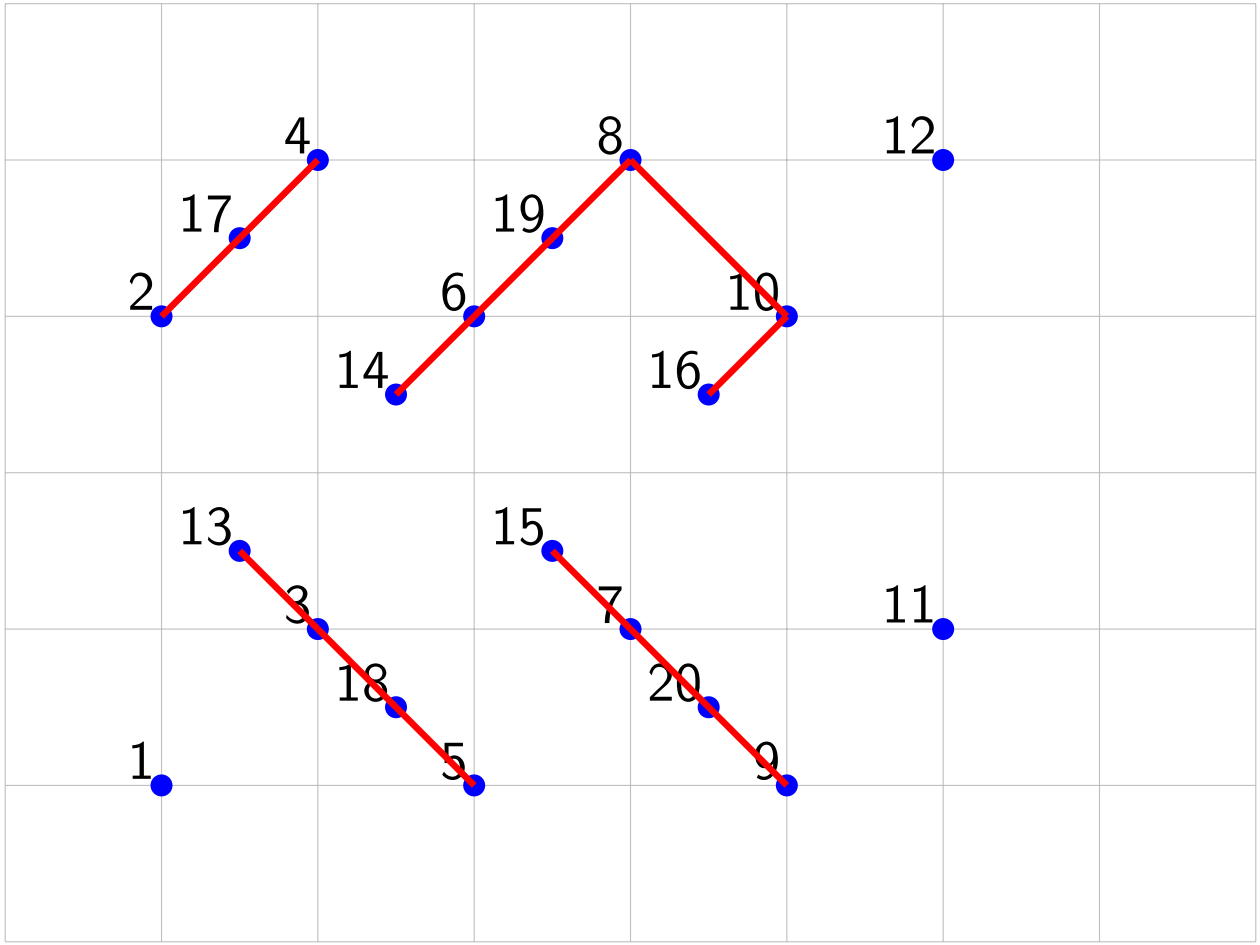
Sorted edges Example

Next cheapest = (5, 7)



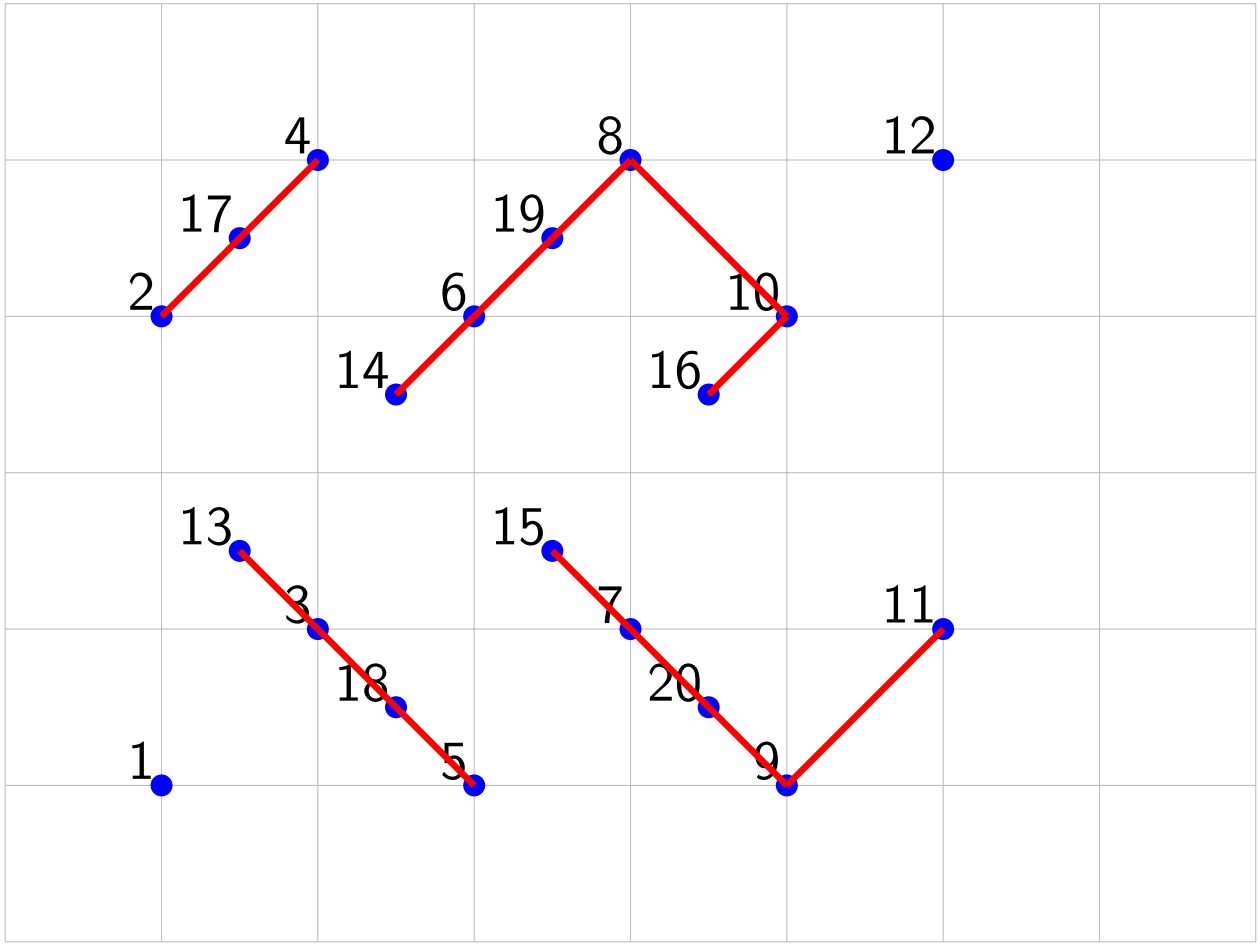
Sorted edges Example

Next cheapest = (8, 10)



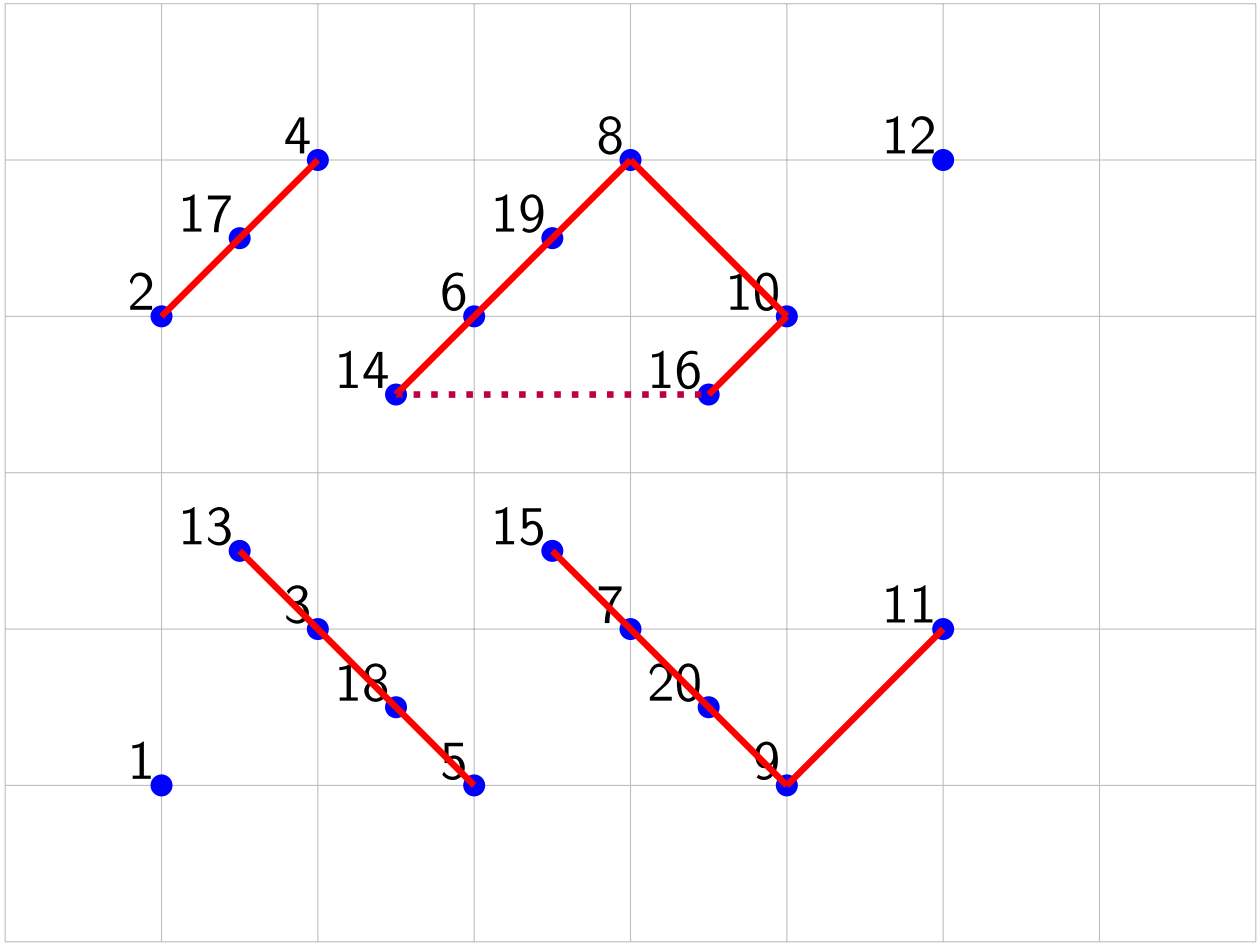
Sorted edges Example

Next cheapest = (9, 11)



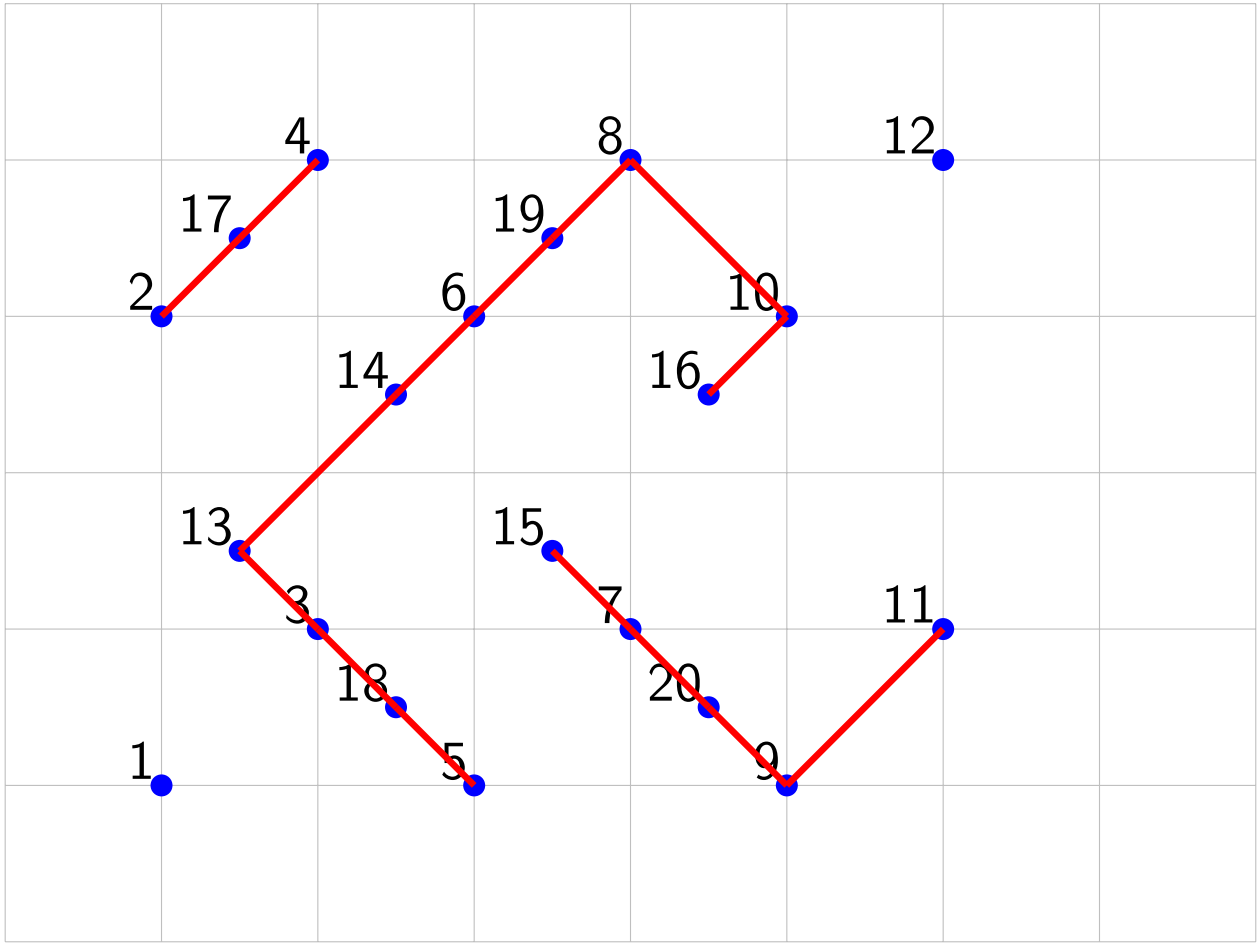
Sorted edges Example

Next cheapest = (14, 16)



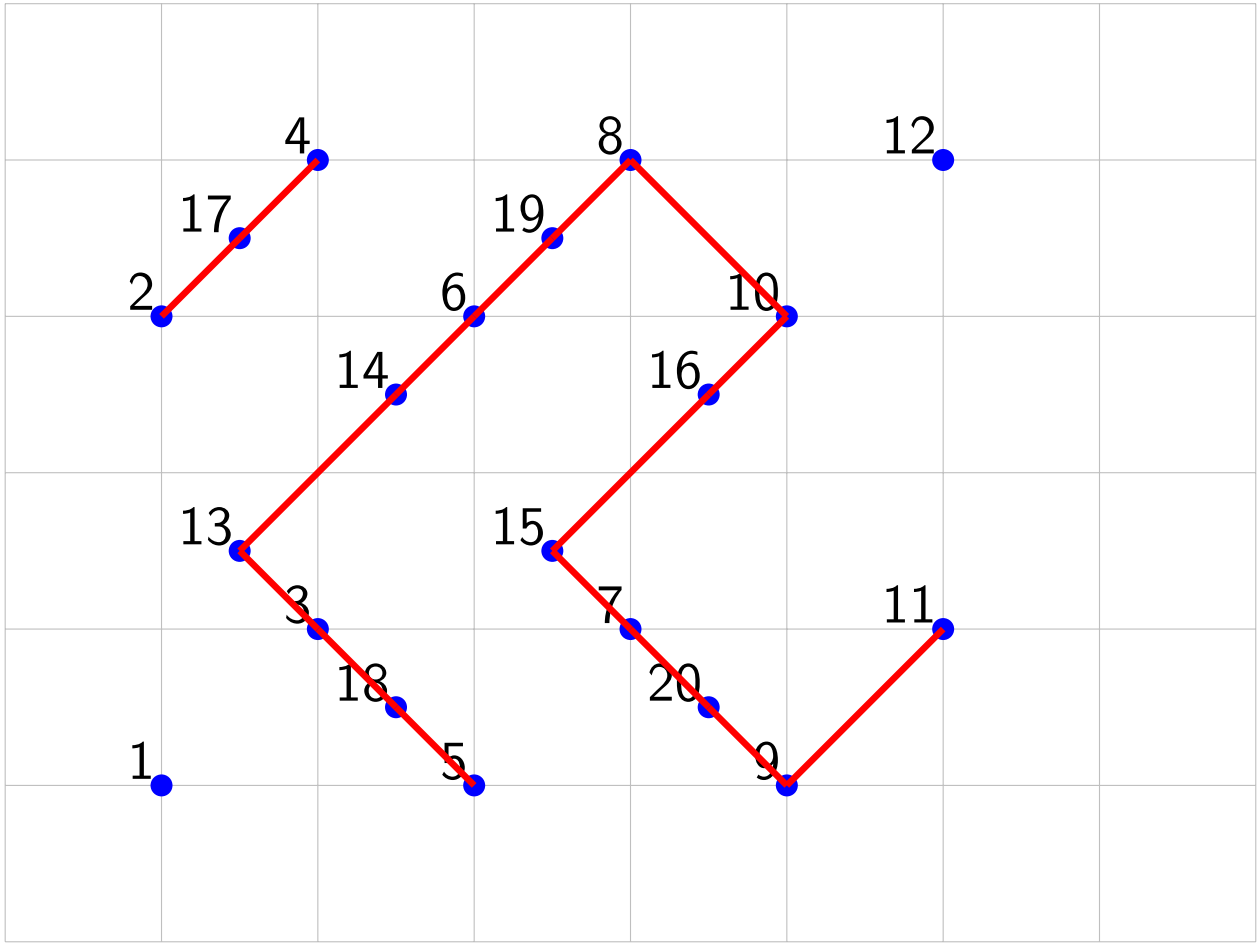
Sorted edges Example

Next cheapest = (13, 14)



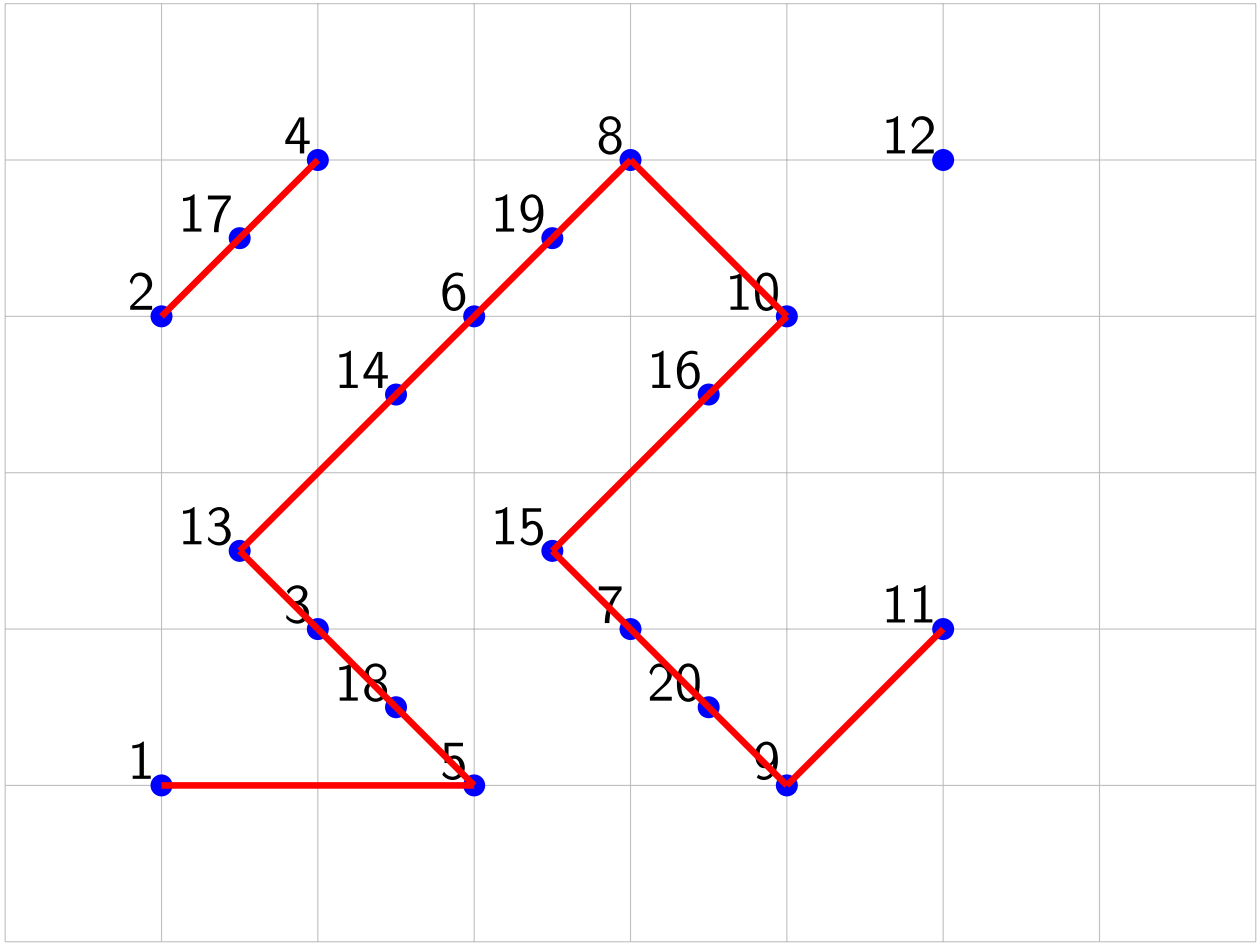
Sorted edges Example

Next cheapest = (15, 16)



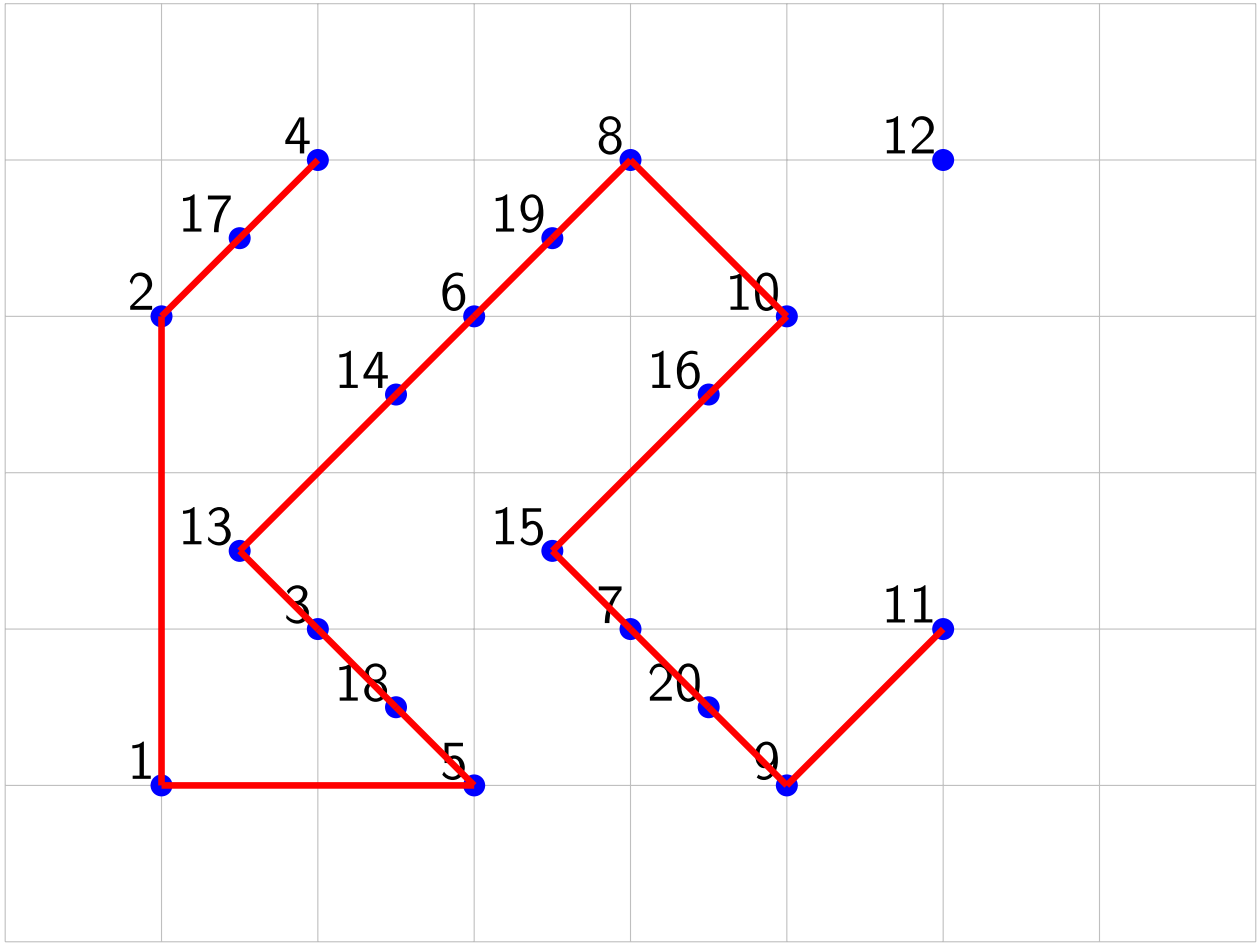
Sorted edges Example

Next cheapest = (1, 5)



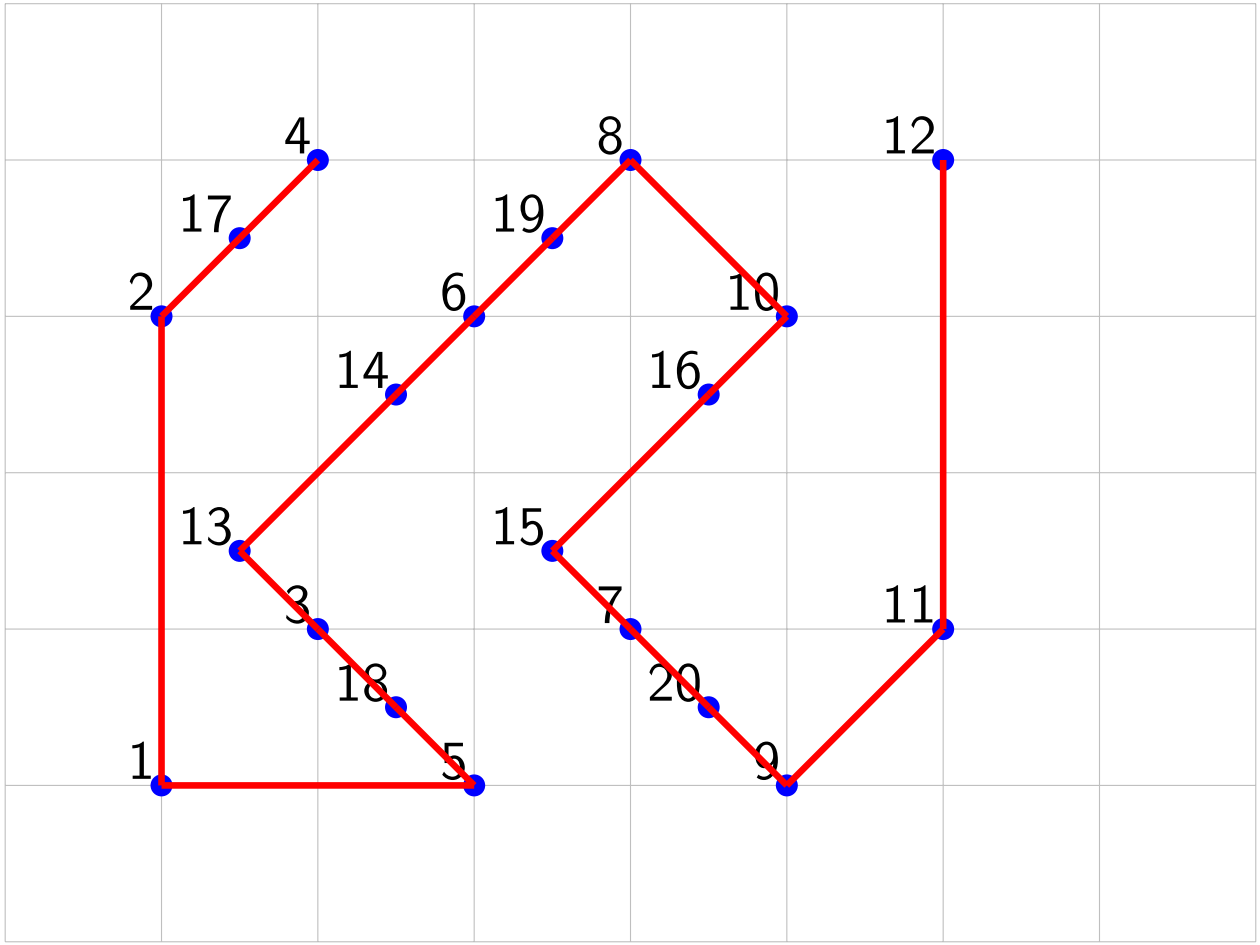
Sorted edges Example

Next cheapest = (1, 2)



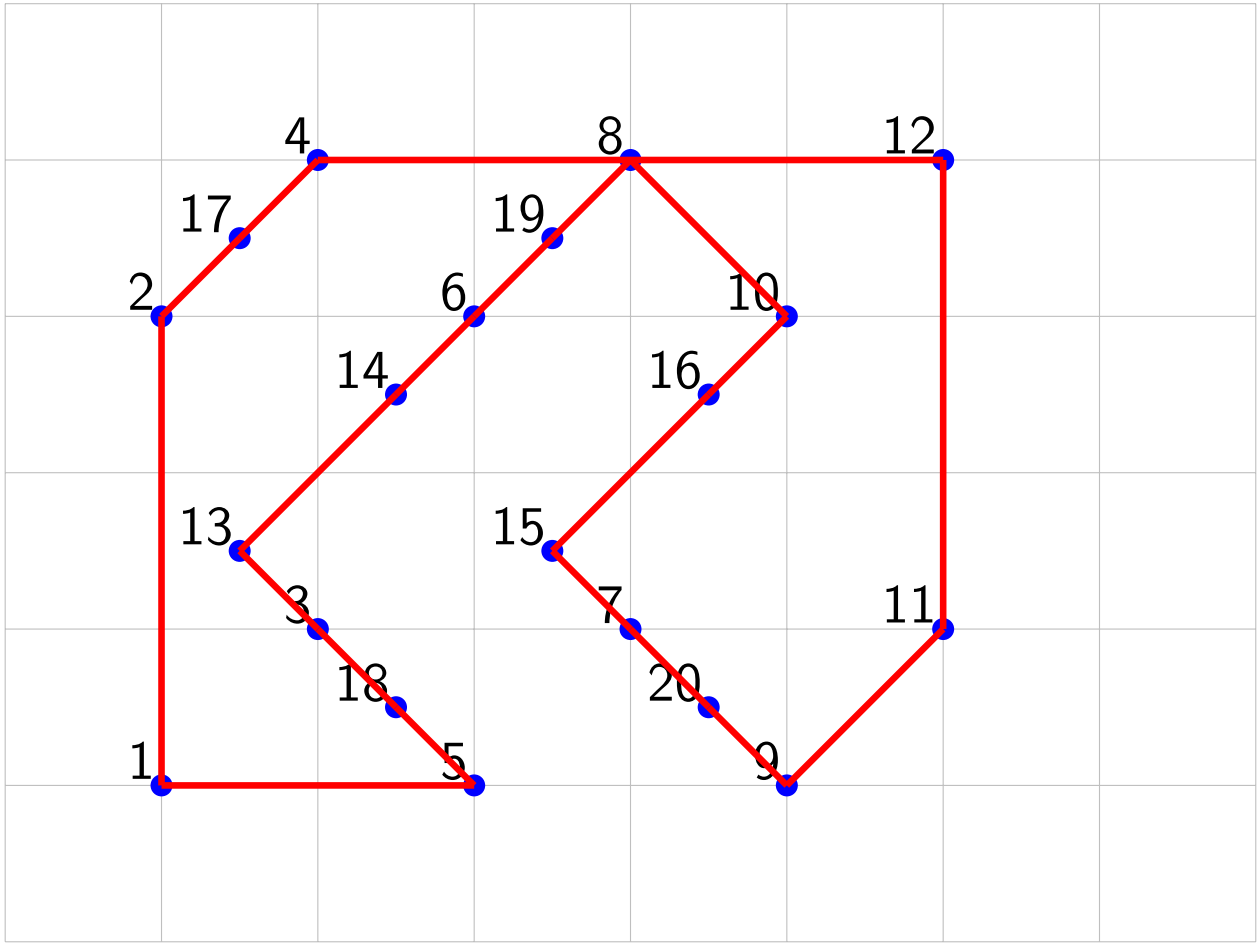
Sorted edges Example

Next cheapest = (11, 12)



Sorted edges Example

Next cheapest = (4, 12). Total cost = 26.142



Sorted edges Example

$$C = \{\{2, 17, 4, 12, 11, 9, 20, 7, 15, 16, 10, 8, 19, 6, 14, 13, 3, 18, 5, 1\}\}$$

$$|C| = 1$$

Evaluation

Which heuristic is better? NN or SE?

$$NN > SE \rightarrow 26.765 > 26.142$$

- This is not always the case;
- If we start the NN in a different city the solution can change;
- When SE heuristic has equal cost edges we can get different solutions based on a random choice.
- **Is there any room for improvement?**

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Evaluation

Is there any room for improvement?

- How do we know that we should invest more time improving our heuristics?
- Is there a simple way to evaluate the solution;
- If we had a good lower bound for the solution then we could compare!

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Evaluation

The optimality gap is the gap between a feasible solution value (upper bound) and a lower bound (relaxation).

$$\frac{UB - LB}{LB} \times 100\%$$

The optimal solution is both an upper bound and a lower bound:

- A feasible solution cannot be lower that the optimal, otherwise the optimal solution would not be optimal;
- The optimal solution is a feasible solution, hence it is also an upper bound.

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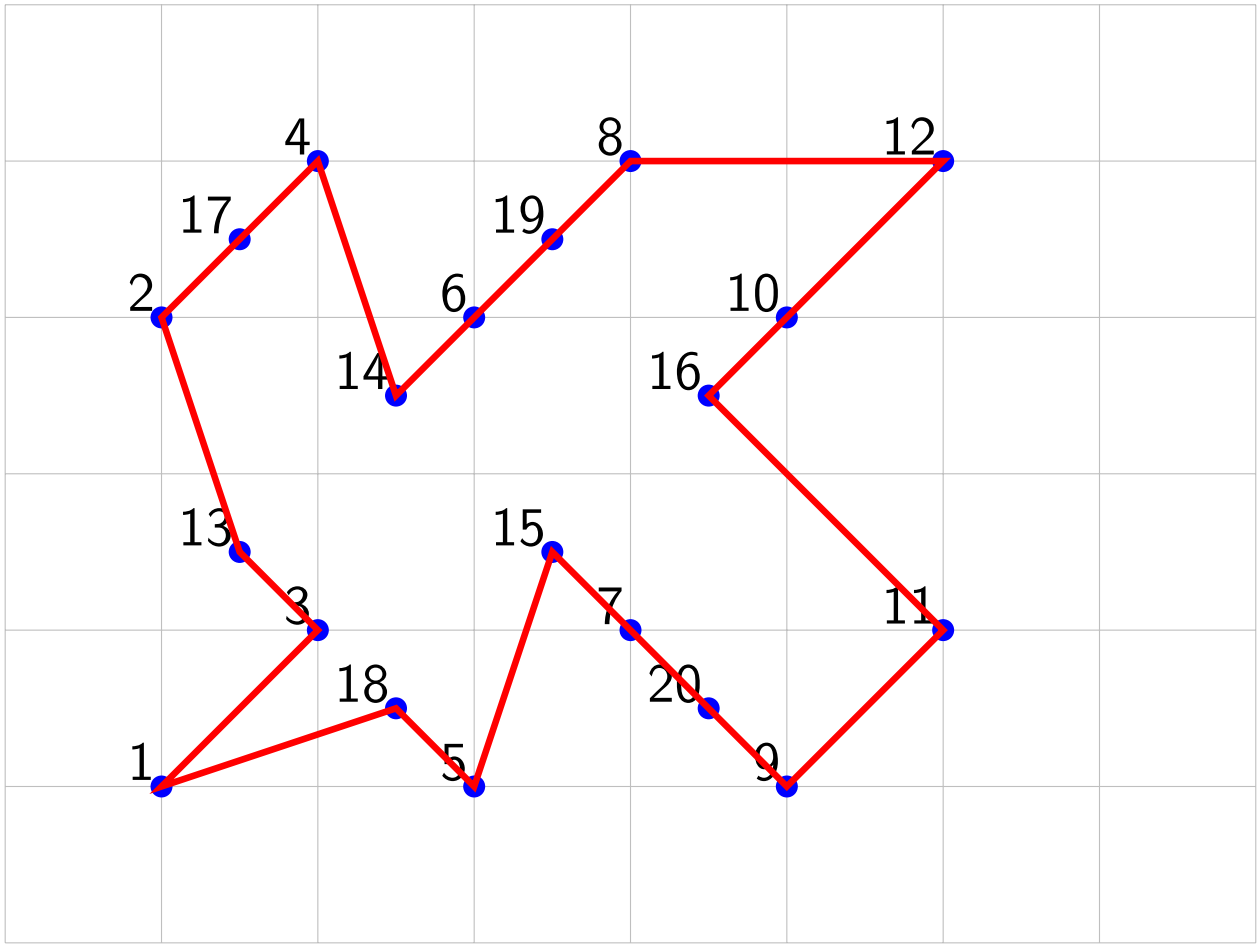
Solution with B&C

Optimal cost = 22.4667



Evaluation

Sorted edges

$$\frac{SE - opt}{opt} \times 100\%$$

$$\frac{26.142 - 22.467}{22.467} \times 100\% \approx 16.36\%$$

Nearest Neighbor

$$\frac{NN - opt}{opt} \times 100\%$$

$$\frac{26.765 - 22.467}{22.467} \times 100\% \approx 19.13\%$$

EPFL

Evaluation

Is a 16.36% gap a "**good**" solution?

- The size and complexity of the problem, as well as the time constraints, can make it necessary to accept a suboptimal solution with a larger gap.
- The cost implications of the suboptimal solution, such as high shipping costs, may require a more accurate solution with a smaller gap.
- The acceptable gap between solutions may vary depending on the level of service quality required or the specific needs of the problem at hand.

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Local Search

Local Search algorithms optimize the cost function by exploring the neighborhood of the current point in the solution space.

- A move is a change in the solution, e.g., swapping customers in a route.
- LS makes a move that improves the solution at each step.
- Once no improving predefined moves exist the algorithm stops (**Local optima**).

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Local Search

Let S be the set of feasible solutions and let f be the objective function of the problem.

- **Definition 1:** Let $\mathcal{H}$ be a heuristic that defines for each solution $w \in S$ a subset $S_w \subseteq S$ of solutions "close" (to be defined by the user according to the problem of interest) to the solution w. The subset S_w is called the neighborhood of solution w.
- **Definition 2:** A solution $w^* \in S$ is called a local optimum with respect to $\mathcal{H}$ for the subset of feasible solutions S and the objective function f if $f(w^*) \leq f(z)$ for all $z \in S_{w^*}$.
- **Definition 3:** The neighborhood structure $\mathcal{H}$ is said to be exact if, for every local optimum with respect to $\mathcal{H}$, $w^* \in S$, w^* is also a global optimum of S and f.

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Local Search Algorithms

Input : Initial solution w
Output: Best solution found
while *termination condition not met* **do**
    Generate a solution z from the neighborhood S_w of the current solution w;
    if $f(z) < f(w)$ **then**
        w $\leftarrow$ z;
    end
    if $f(z) \geq f(w)$ *for all* $z \in S_w$ **then**
        Terminate;
    end
end

Algorithm 1: Local Search

EPFL

k-opt

- The **k-opt** algorithm is a **local search** algorithm for the **Traveling Salesman Problem (TSP)**.
- The algorithm works by iteratively improving a **feasible solution** to the TSP by exploring its **neighborhood** using a **k-opt move**.
- The **k-opt move** involves removing **k** edges from the current solution and reconnecting the resulting fragments in a new way to obtain a new feasible solution.
- The value of **k** determines the size of the neighborhood and the complexity of the search.
- The algorithm terminates when no further improvement can be made, and the current solution is returned as the approximate solution to the TSP.

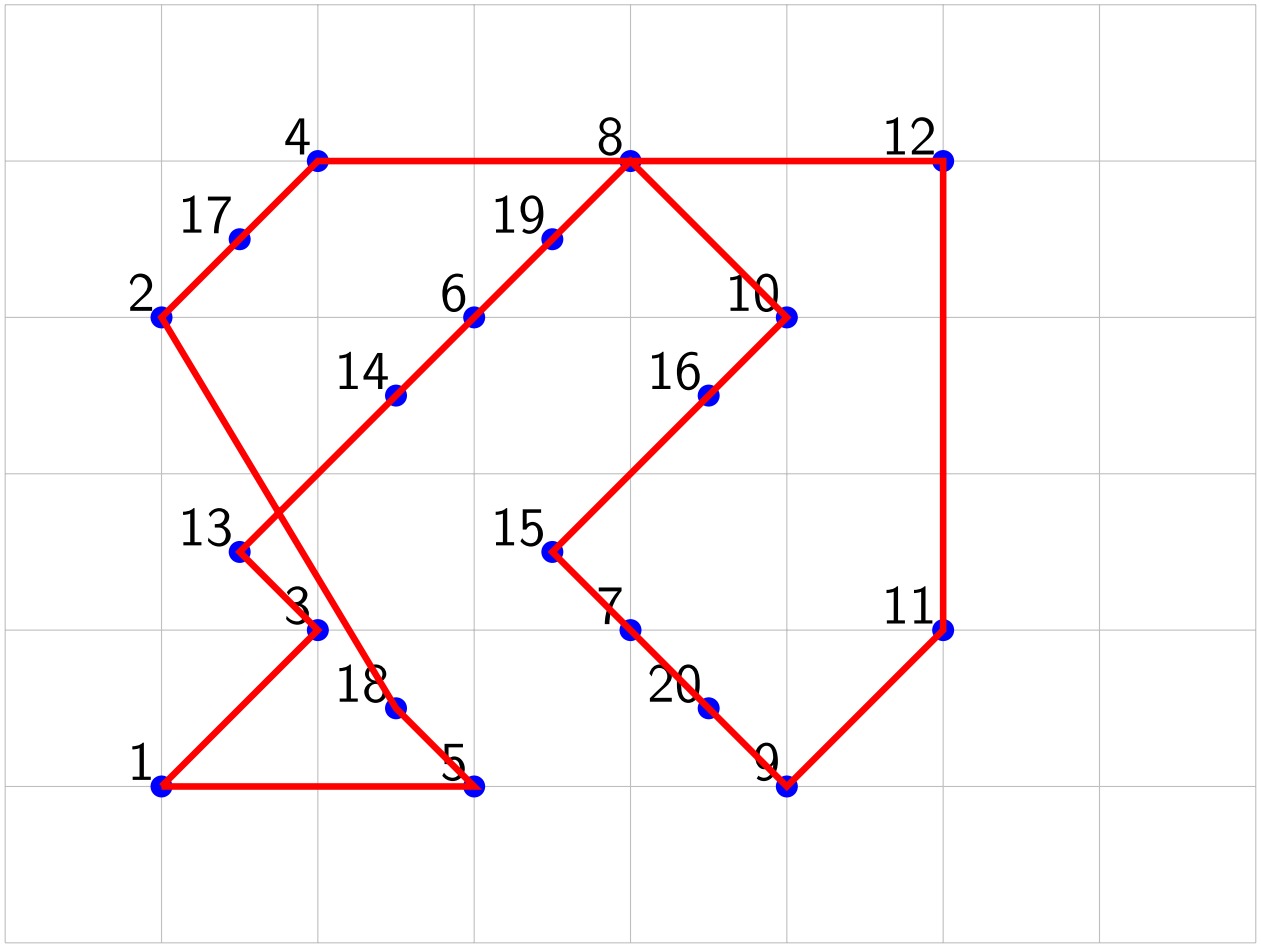
2-opt algorithm

Input : An initial tour T for the TSP
Output: An approximate solution to the TSP
Set $T^* \leftarrow T$;
while *no improvement is made* **do**
  for $i \in T^*$ **do**
    for $j = i + 1$ **to** $|T|$ **do**
      if $d_{i,i-1} + d_{j+1,j} > d_{i,j+1} + d_{i-1,j}$ **then**
        $R \leftarrow$ Reverse the segment between cities $i - 1$ and $j + 1$;
        $T^* \leftarrow R$;
      end
    end
  end
end

Algorithm 2: 2-opt algorithm for TSP

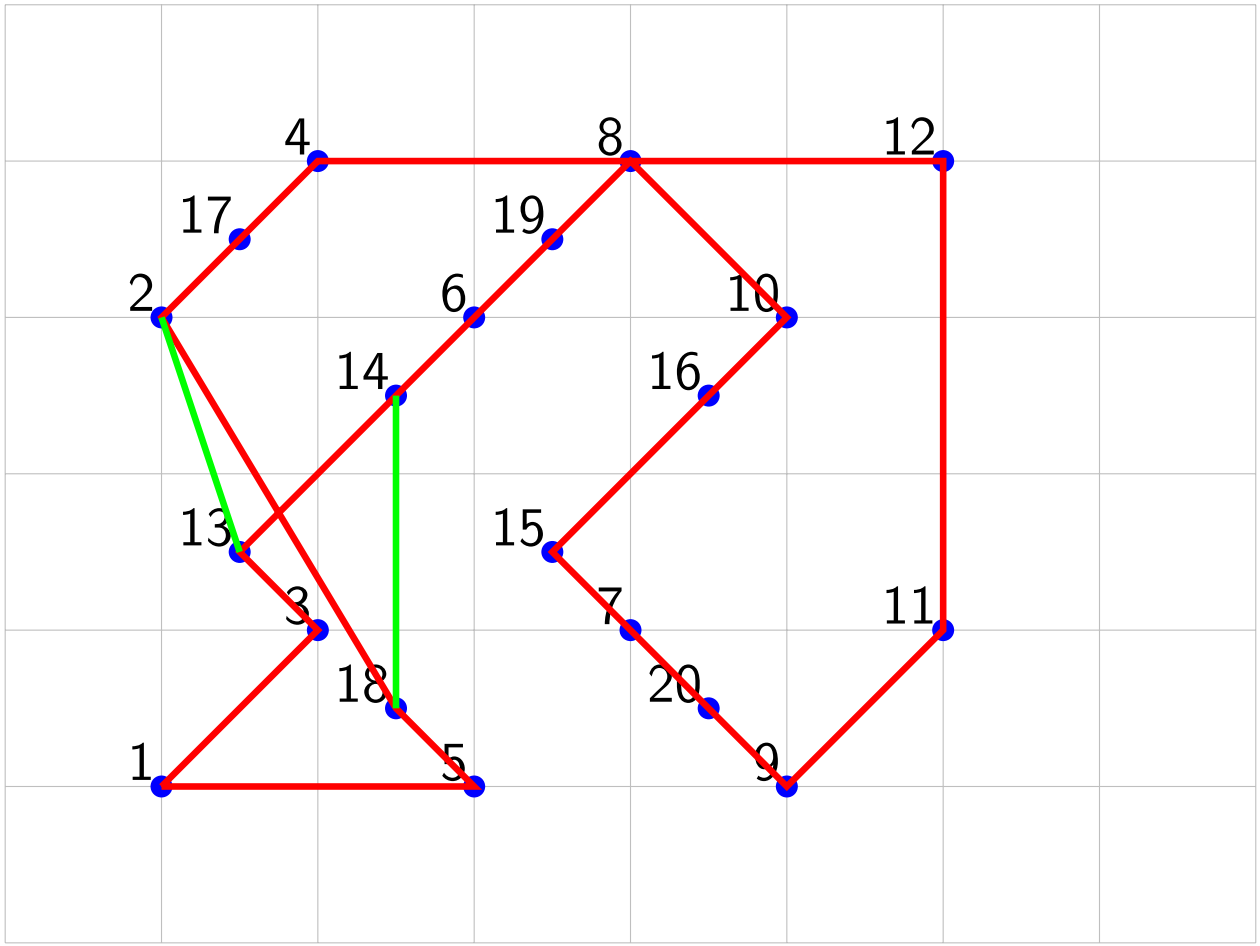
2-opt Example

Initial tour is the NN solution



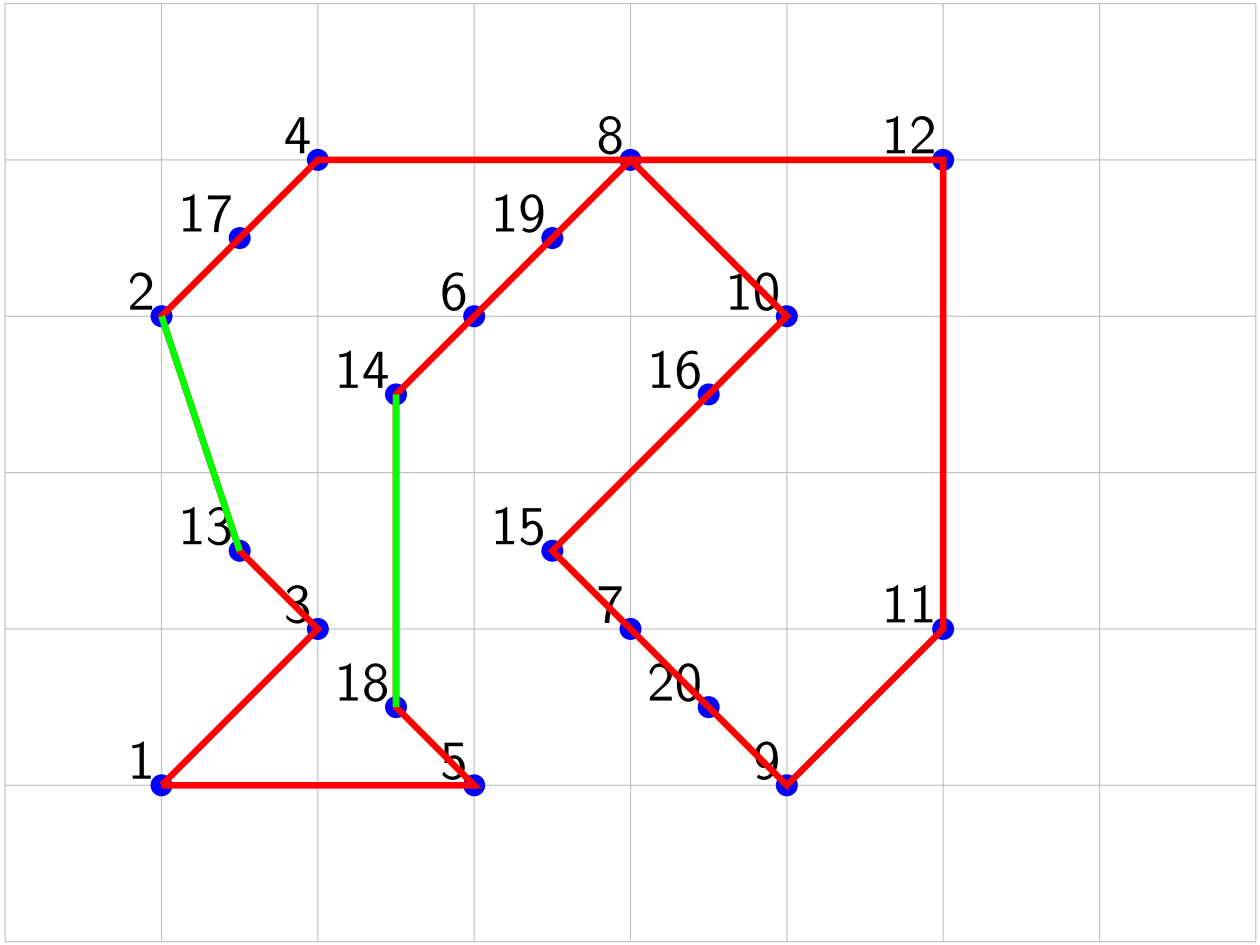
2-opt Example

A 2-opt move consists of replacing 2 edges with 2 new edges



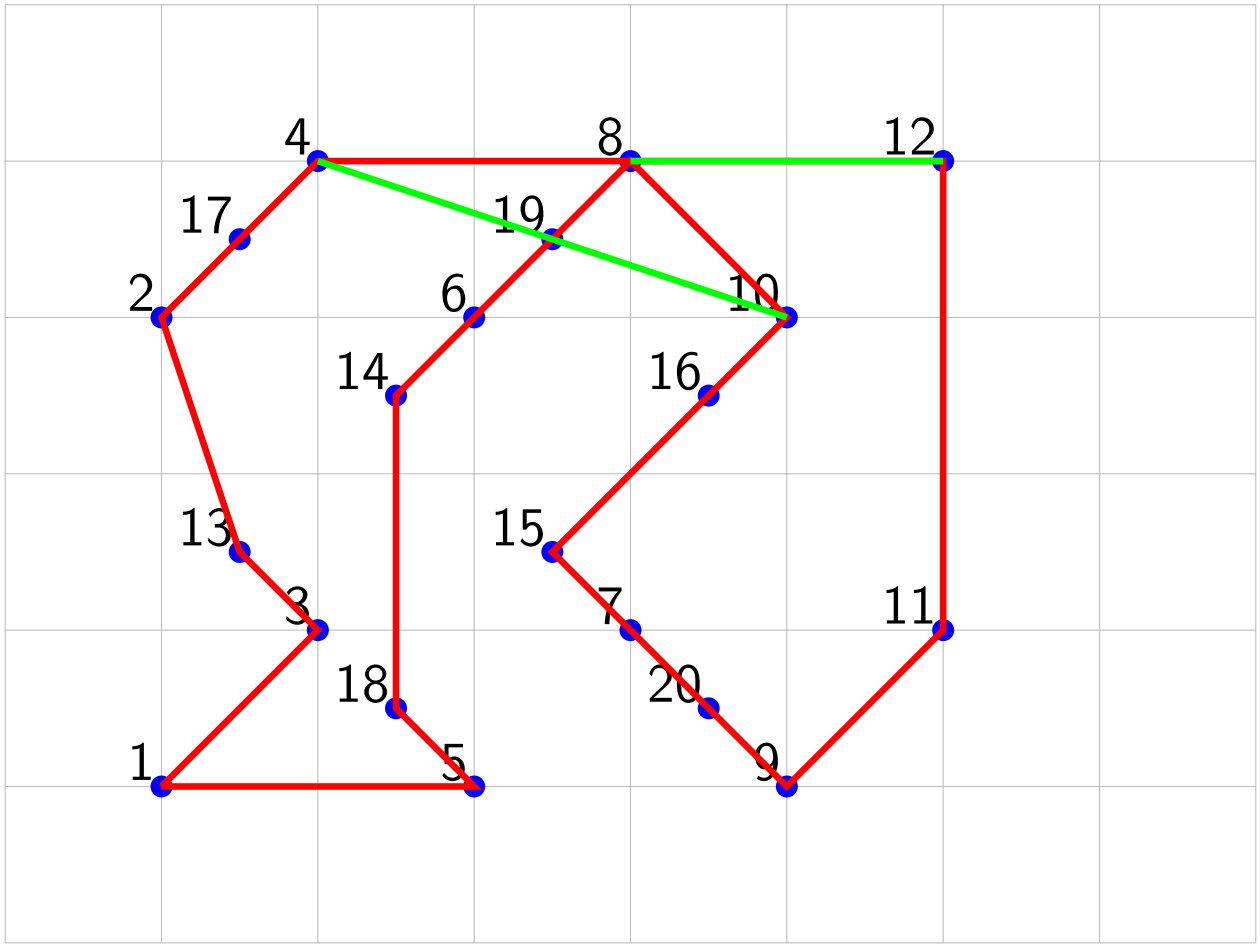
2-opt Example

Remove (13,14) and (2,18). Now add (2,13) and (14,18) to reconnect the tour.

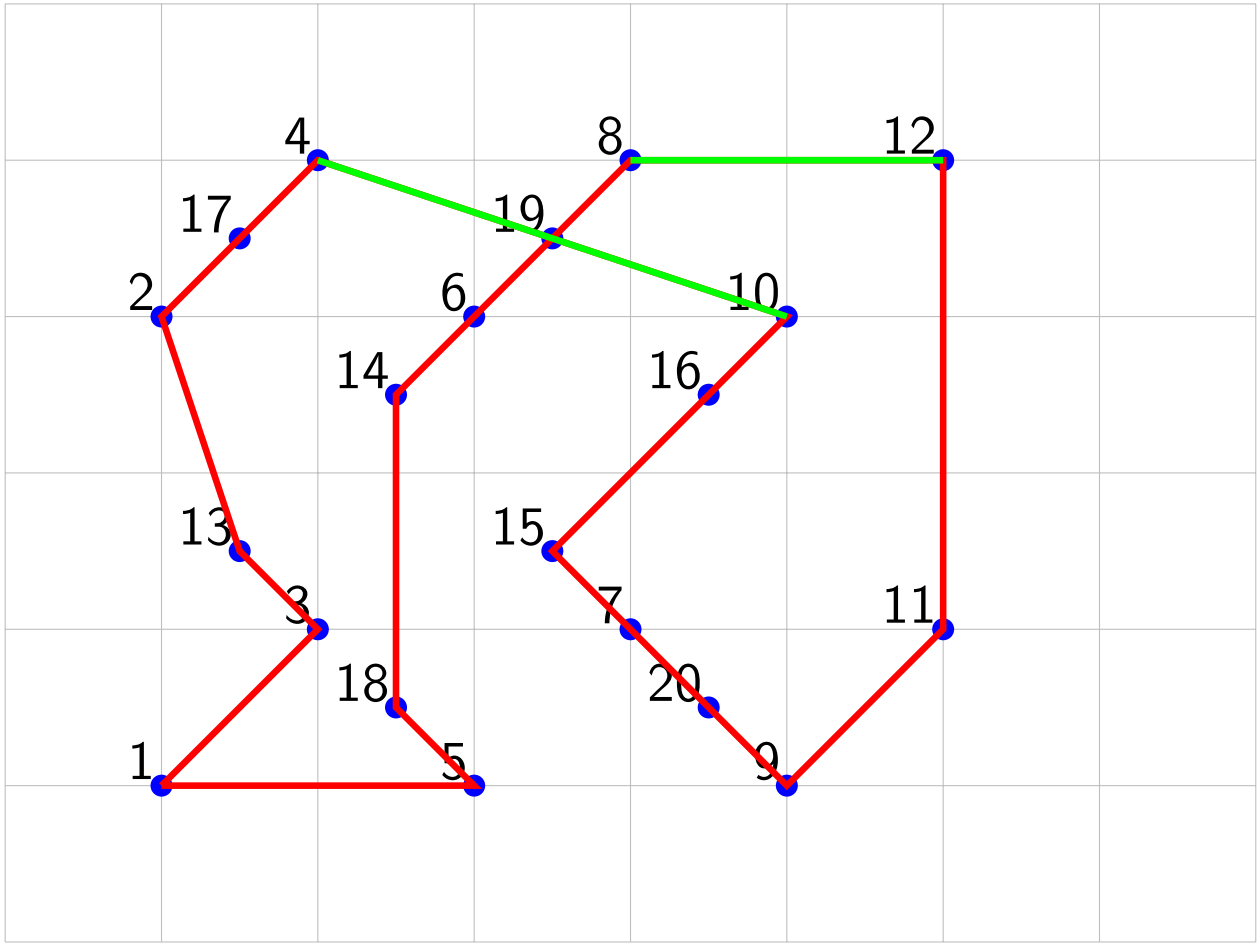


2-opt Example

2-opt continues only making moves that improve the objective function.

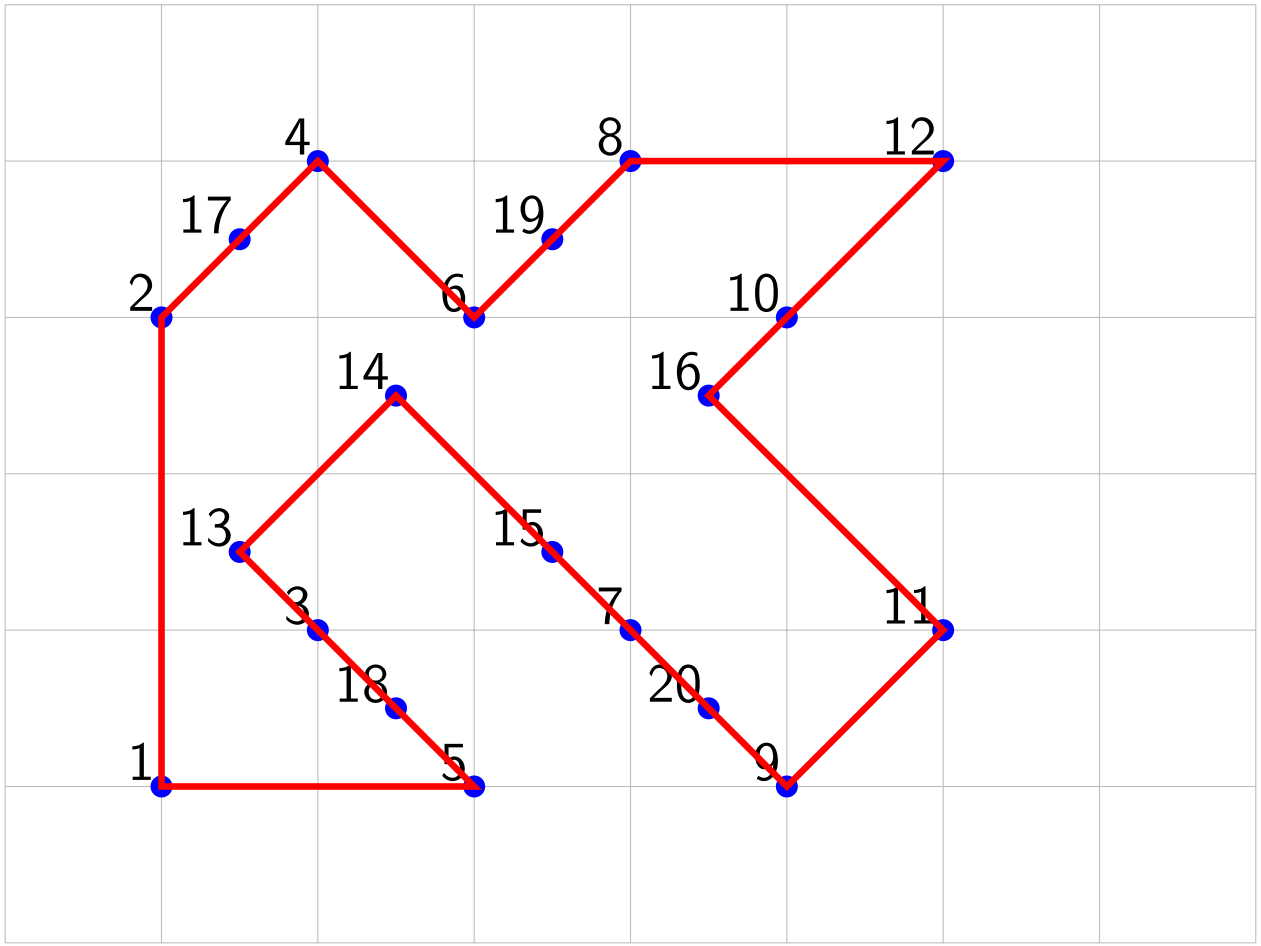


2-opt Example



2-opt Example

2-opt solution value = 23.97. **Local optimum**



Evaluation

Is this solution better?

$$\frac{2opt - opt}{opt} \times 100\%$$

$$\frac{23.97 - 22.467}{22.467} \times 100\% \approx 6.72\%$$

Why not do 10-opt or more?

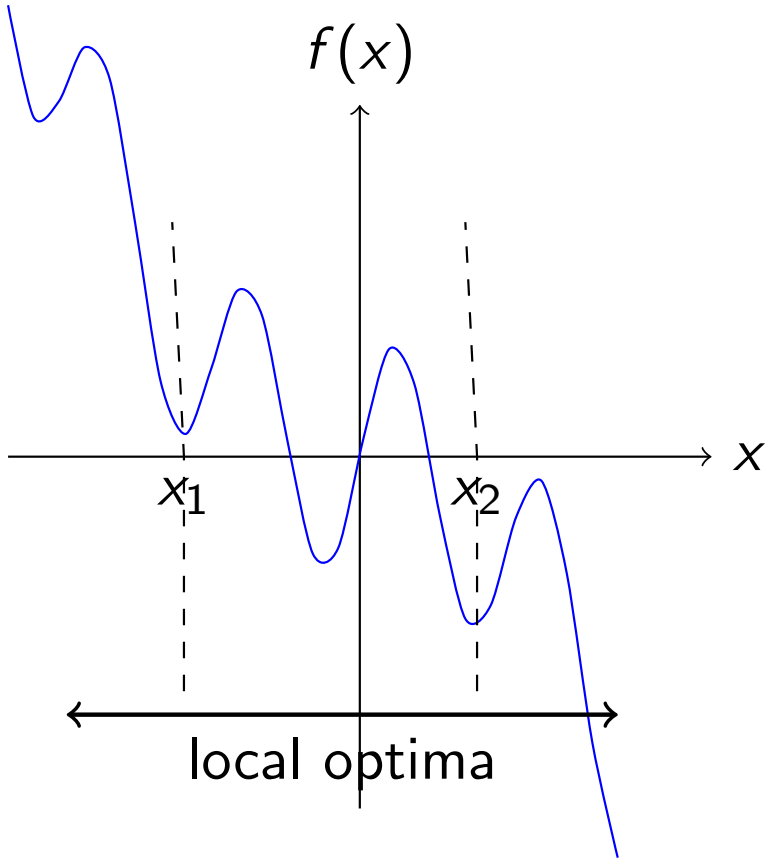
- The time complexity of each iteration for the k-opt algorithm is:

$$\mathcal{O}(n^k)$$

In general, the time complexity of the k-opt algorithm increases exponentially with the value of k, so it is often used with small values of k (such as 2 or 3) to balance between solution quality and computation time.

Local Search

- In a local optimal point there is no descent direction. That is, there is no improving solution in the neighborhood around the current solution



Local Search

- In Local search the local optima is defined by the heuristic (e.g., 2-opt heuristic).
- Once the heuristic cannot identify an improving move, then we say that the solution is a local optima (e.g., 2-opt local optima).
- Notice that if we change the heuristic (e.g, 4-opt) we could improve the solution to arrive at a new local optima for the new heuristic.
- **Disadvantage** local search is unable to escape local optima since it does not accept non improving solutions.

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Outline

Metaheuristics

- The idea is to escape local optima by altering the solution in some way (sometimes called kick, shake or destroy).
- Moves that cause an increase in the function can be accepted to escape local optima.
- Once the solution has been altered in some way that is sufficient to escape, local search is used again to improve the new solution.
- Generally, the procedure is repeated for some pre-specified number of iterations.

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Annealing

- Annealing is a process of heating and cooling a material to change its properties.
- It is commonly used in the manufacturing of metals and glass.
- The annealing process involves heating the material to a high temperature, then allowing it to cool slowly.
- This slow cooling allows the material's atoms to rearrange themselves into a more stable configuration.
- Annealing can result in changes to the physical and mechanical properties of a material, such as strength, ductility, and toughness.
- It can also be used to relieve stresses in a material that occur during processes such as welding or machining.

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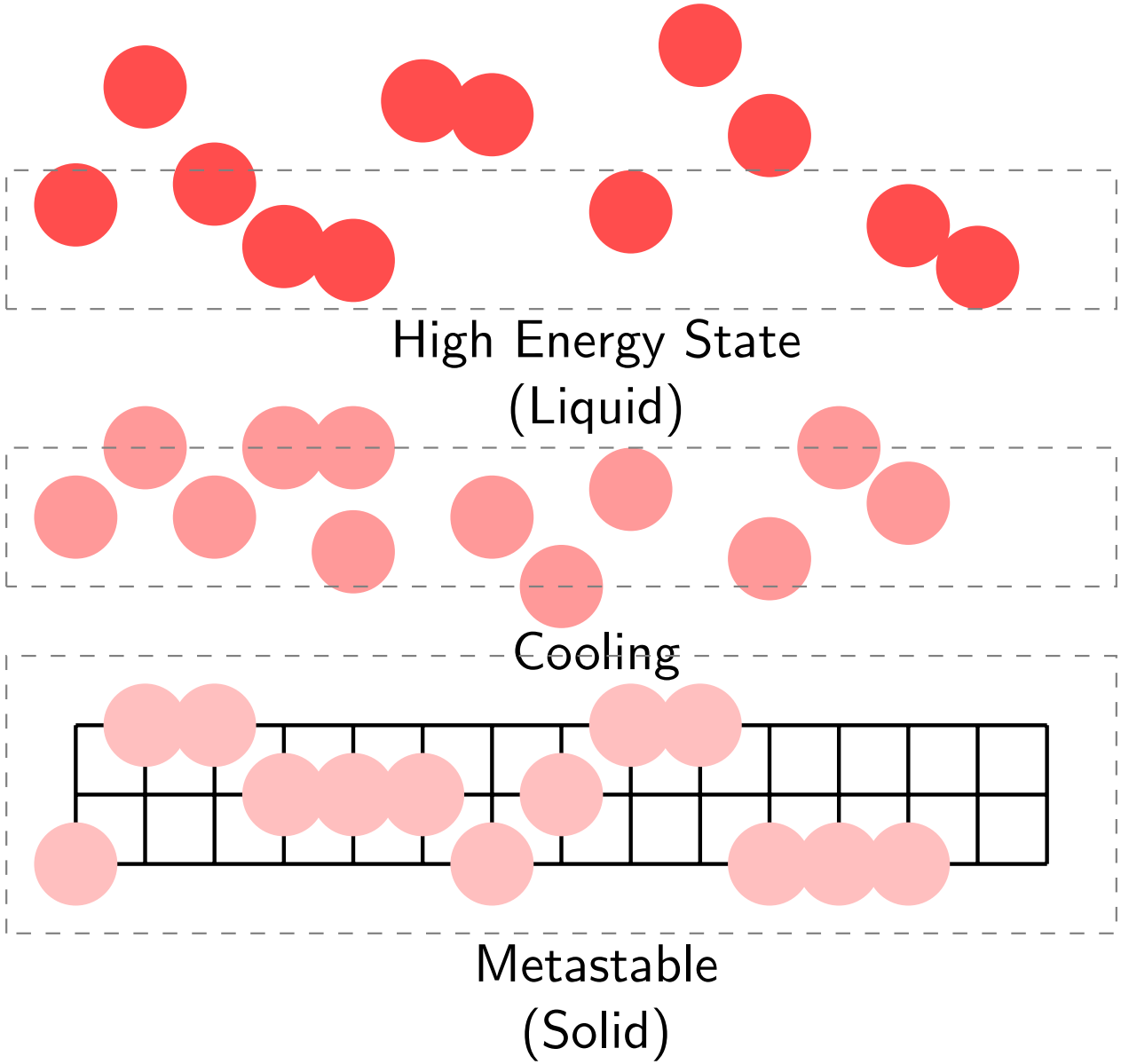
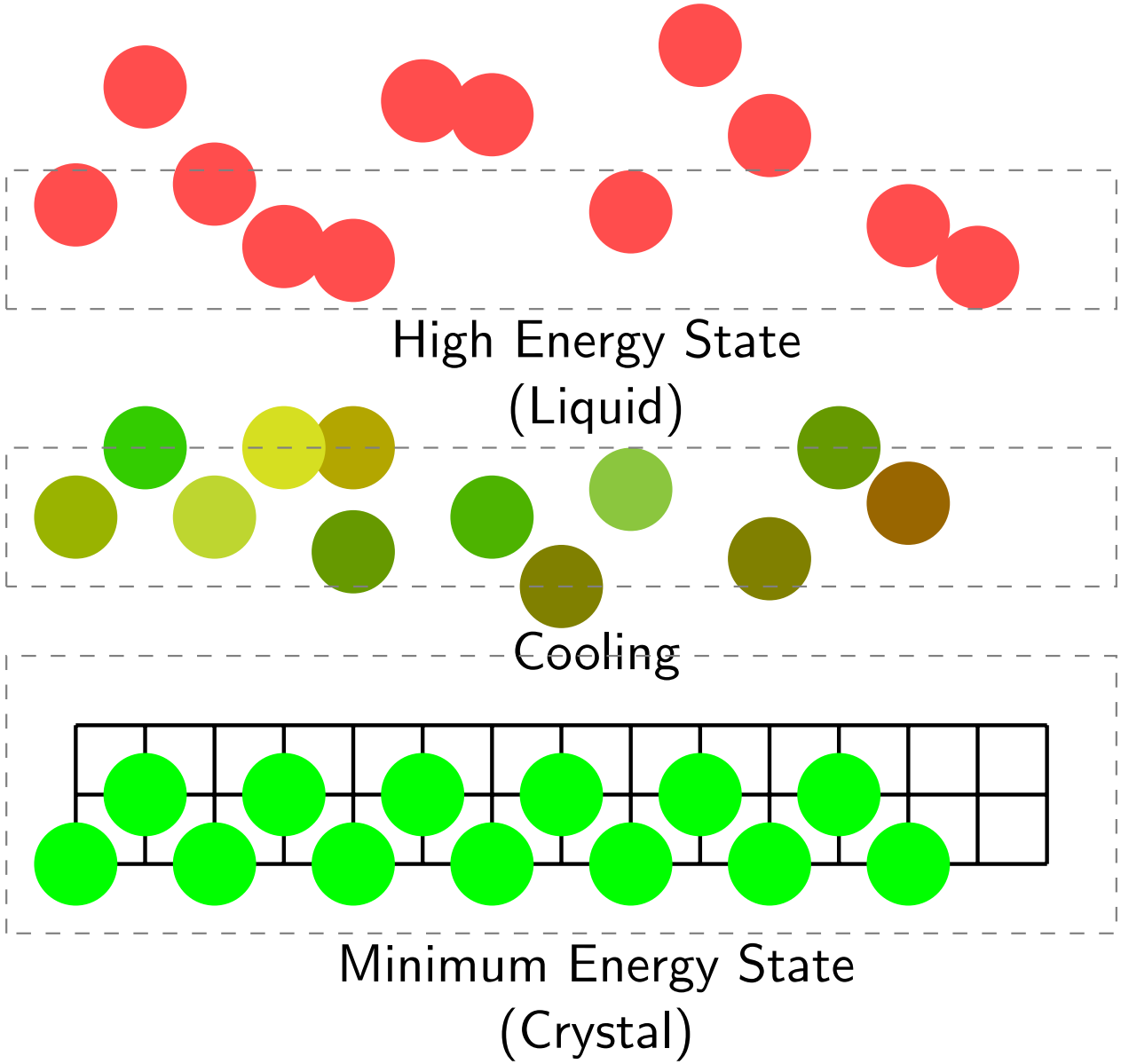
Annealing: Rapid cooling



Annealing: Slow gradual cooling



Simulated Annealing(SA)

- SA is a metaheuristic optimization algorithm based on the physical process of annealing in materials.
- The SA process involves starting with an initial solution and gradually modifying it by changing some elements of the solution.
- At each step, the new solution is evaluated and accepted or rejected based on a probability that depends on the difference between the energy of the new solution and the energy of the current solution, as well as the current temperature.
- Initially, the temperature is set high so that the system is in a high-energy state, allowing for a more complete exploration of the solution space.
- As the temperature is gradually decreased, the system is encouraged to settle into a lower-energy state.
- If the temperature decreases too quickly, the system can become trapped in a local optimum, known as hardening.

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Simulated Annealing

- Let the temperature be $\mathcal{T}$;
- Let $f(z)$ be the new solution's objective value;
- Let $f(w)$ be the current solution's objective value;
- Let $\Pr\{\text{accept } z\}$ be the probability of accepting z as a new current solution.

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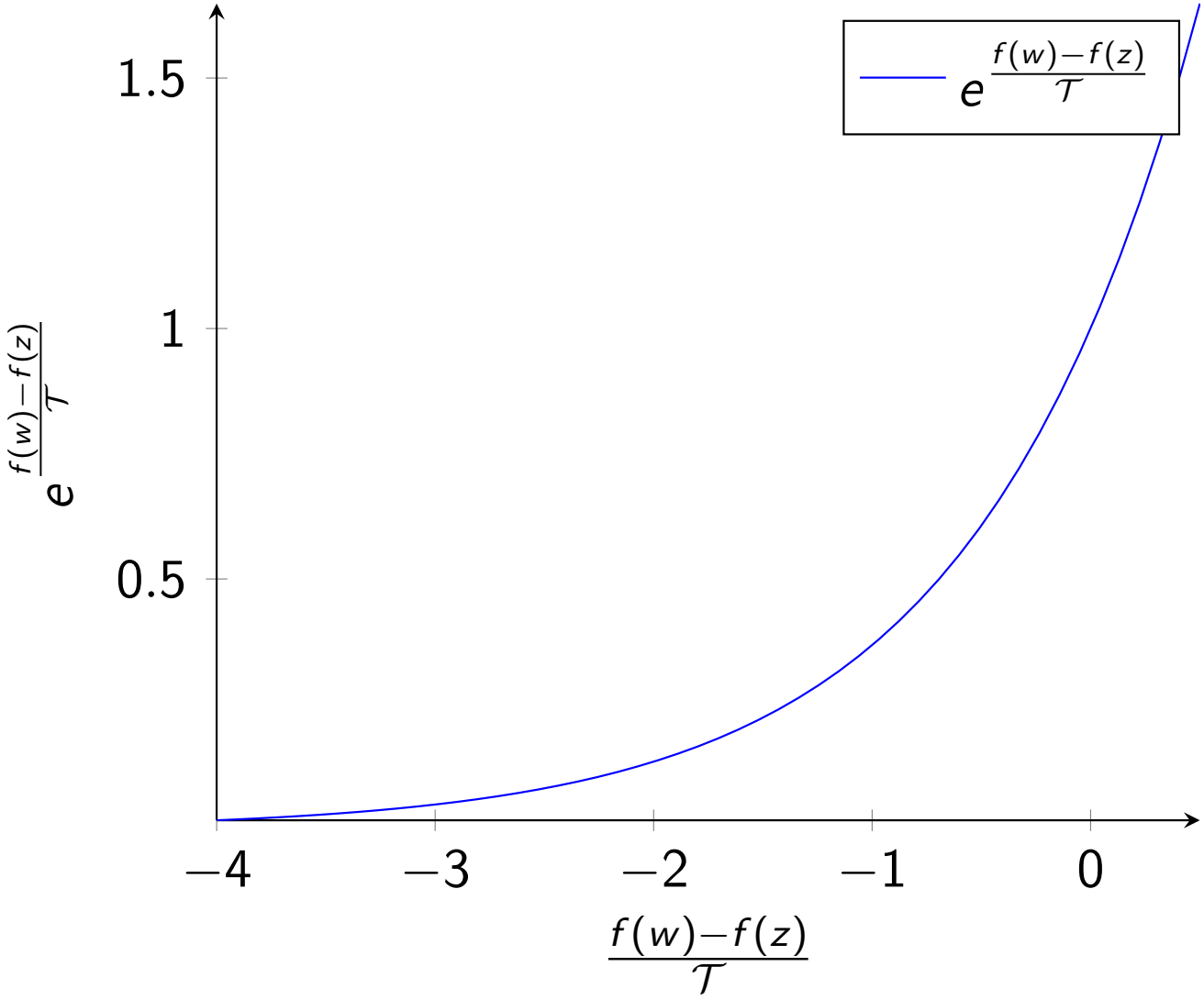
Simulated Annealing

Probability of accepting a new solution:

$$e^{\frac{f(w)-f(z)}{\mathcal{T}}}$$

$$\Pr\{\text{accept } z\} = \begin{cases} 1 & \text{if } f(z) < f(w) \\ e^{\frac{f(w)-f(z)}{\mathcal{T}}} & \text{otherwise} \end{cases}$$

Simulated Annealing



Simulated Annealing

Input : w_{start}, $\mathcal{T}_0$, L_0
Output: Best solution found

$w \leftarrow w_{start}$, $k \leftarrow 0$, $\mathcal{T}_k \leftarrow \mathcal{T}_0$, $L_k \leftarrow L_0$;
while $\mathcal{T}_k \not\approx 0$ **do**
  for $l = 0$ **to** L_k **do**
    Generate a solution z from the neighborhood S_w;
    if $f(z) < f(w)$ **then**
      $w \leftarrow z$;
    end
    else
      Accept z as the current solution with probability $e^{\frac{f(w)-f(z)}{\mathcal{T}_k}}$;
    end
  end
  $k \leftarrow k + 1$;
  Compute $(L_k, \mathcal{T}_k)$;
end
return w;

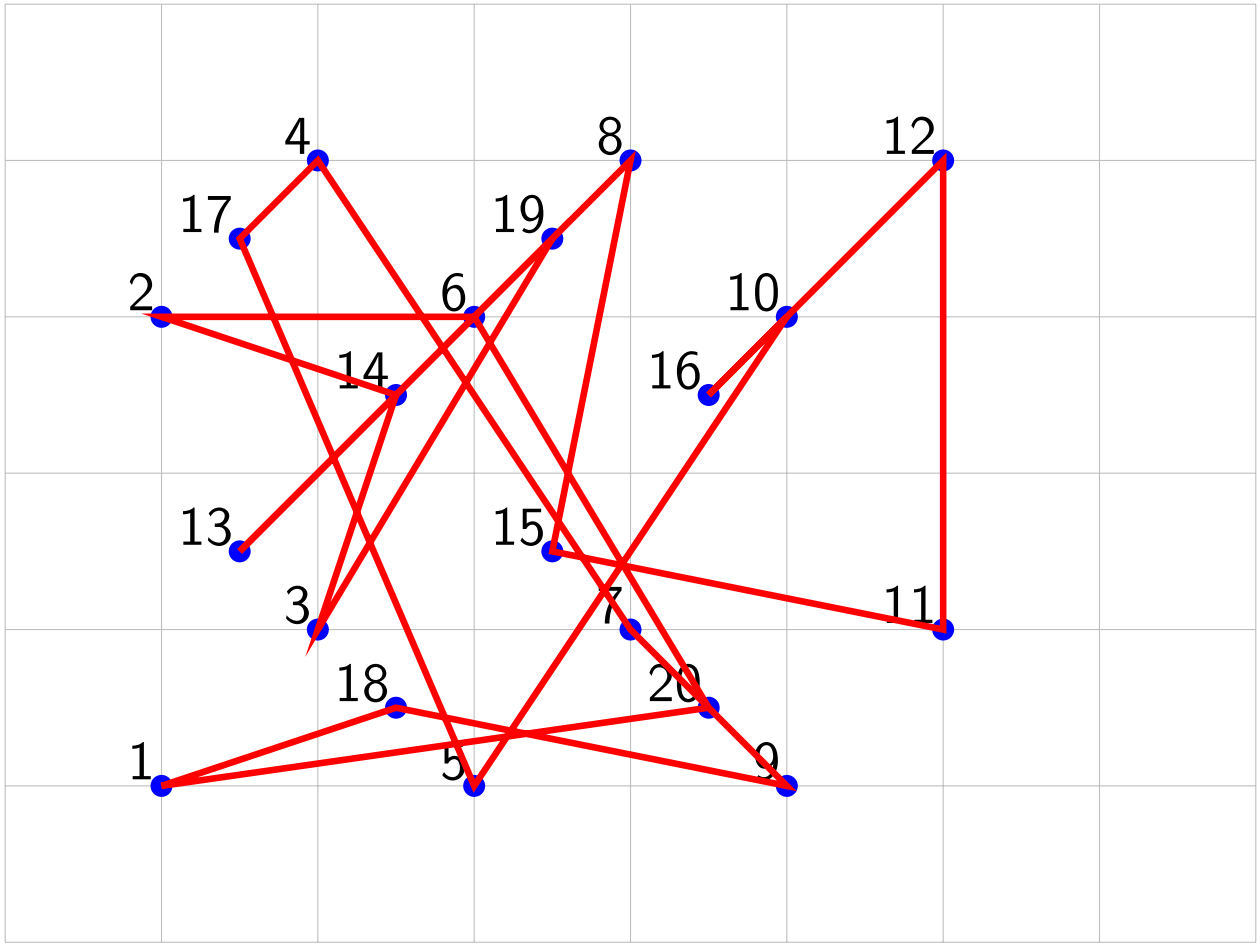
Simulated Annealing

- At each iteration, the algorithm cools the temperature by a cooling factor of α.

$$\mathcal{T}_{k+1} \leftarrow \alpha \times \mathcal{T}_k$$

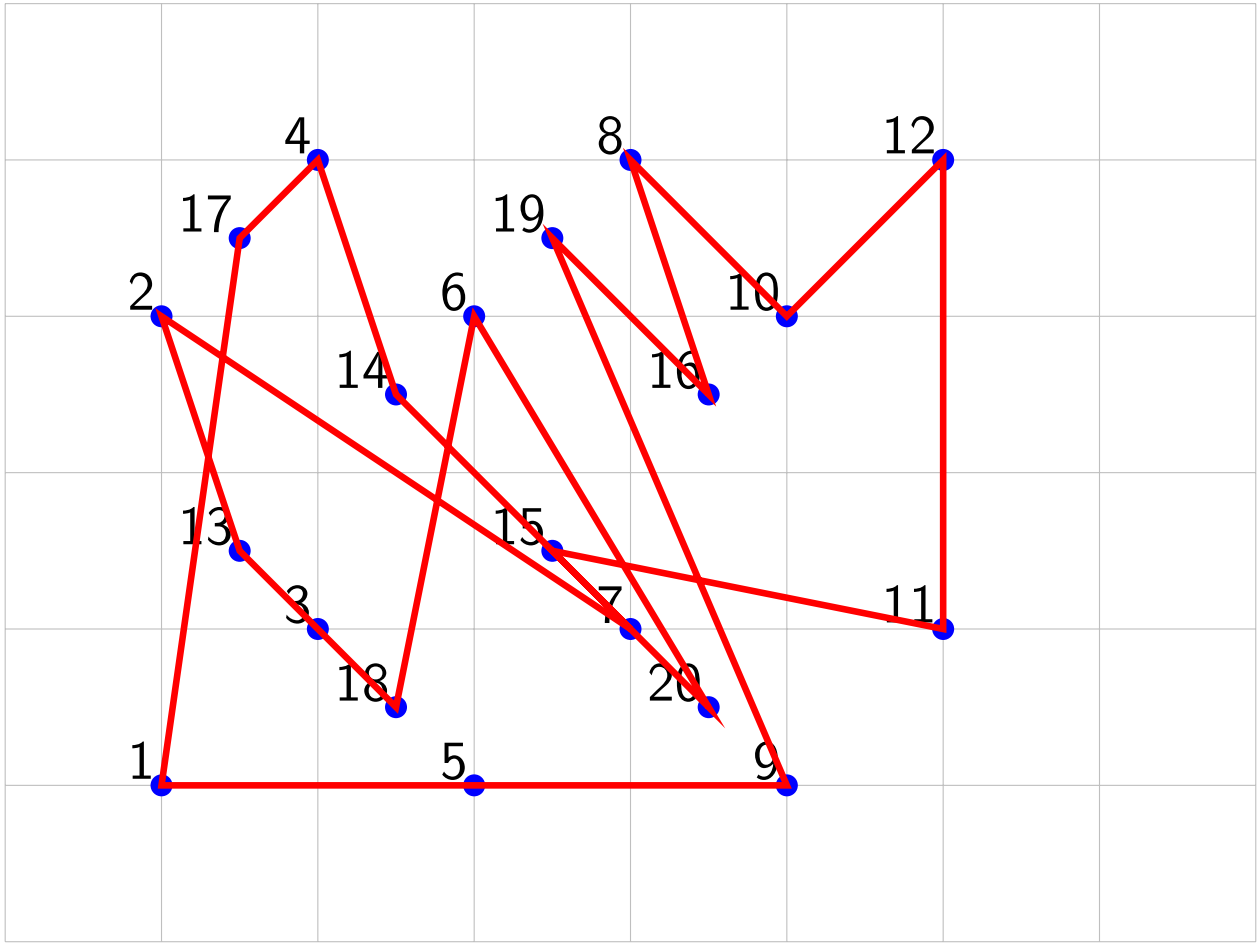
SA Example

$\mathcal{T}_0 = 1000,\ \alpha = 0.999,\ L = 5$



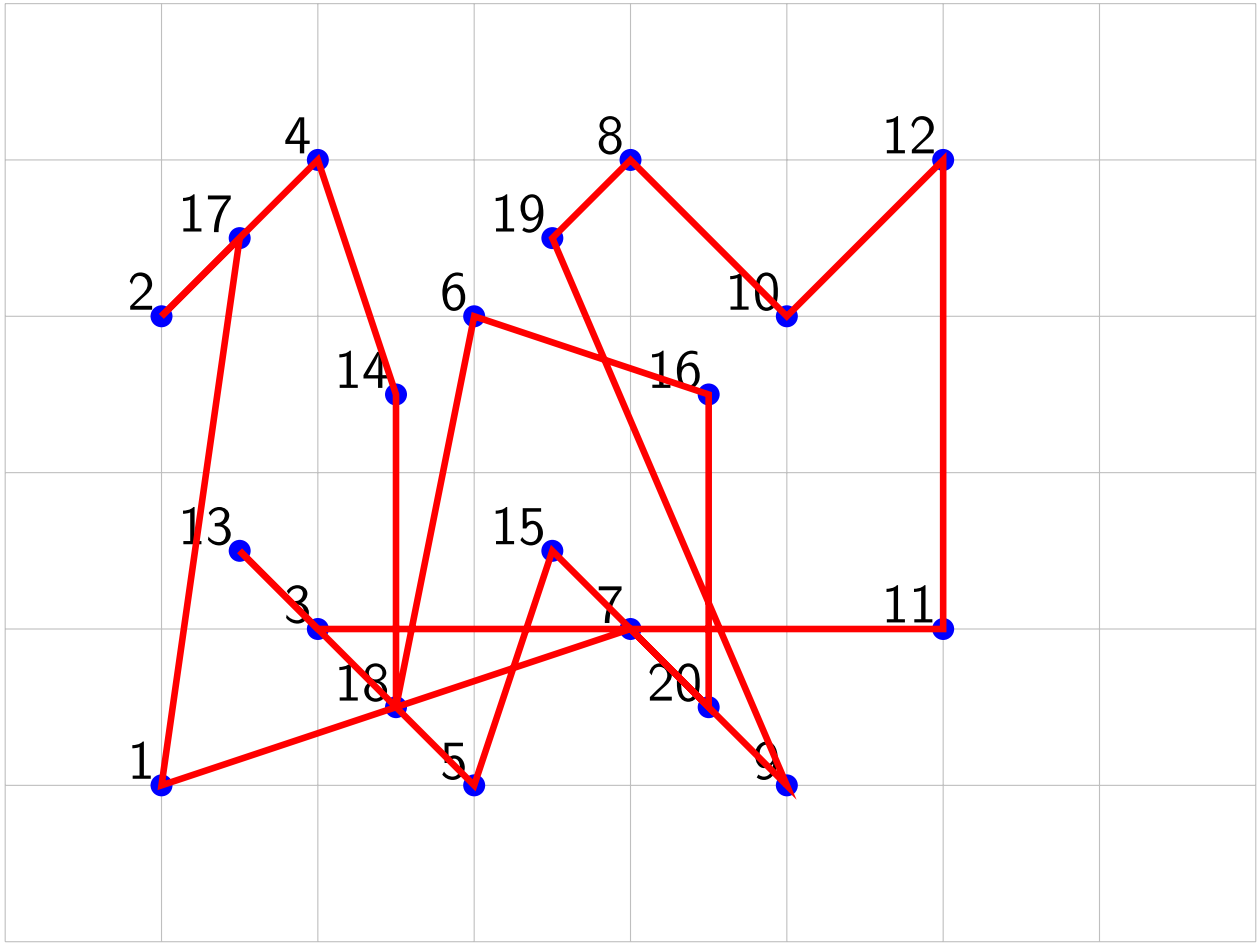
SA Example

$\mathcal{T}_k = 499.9$



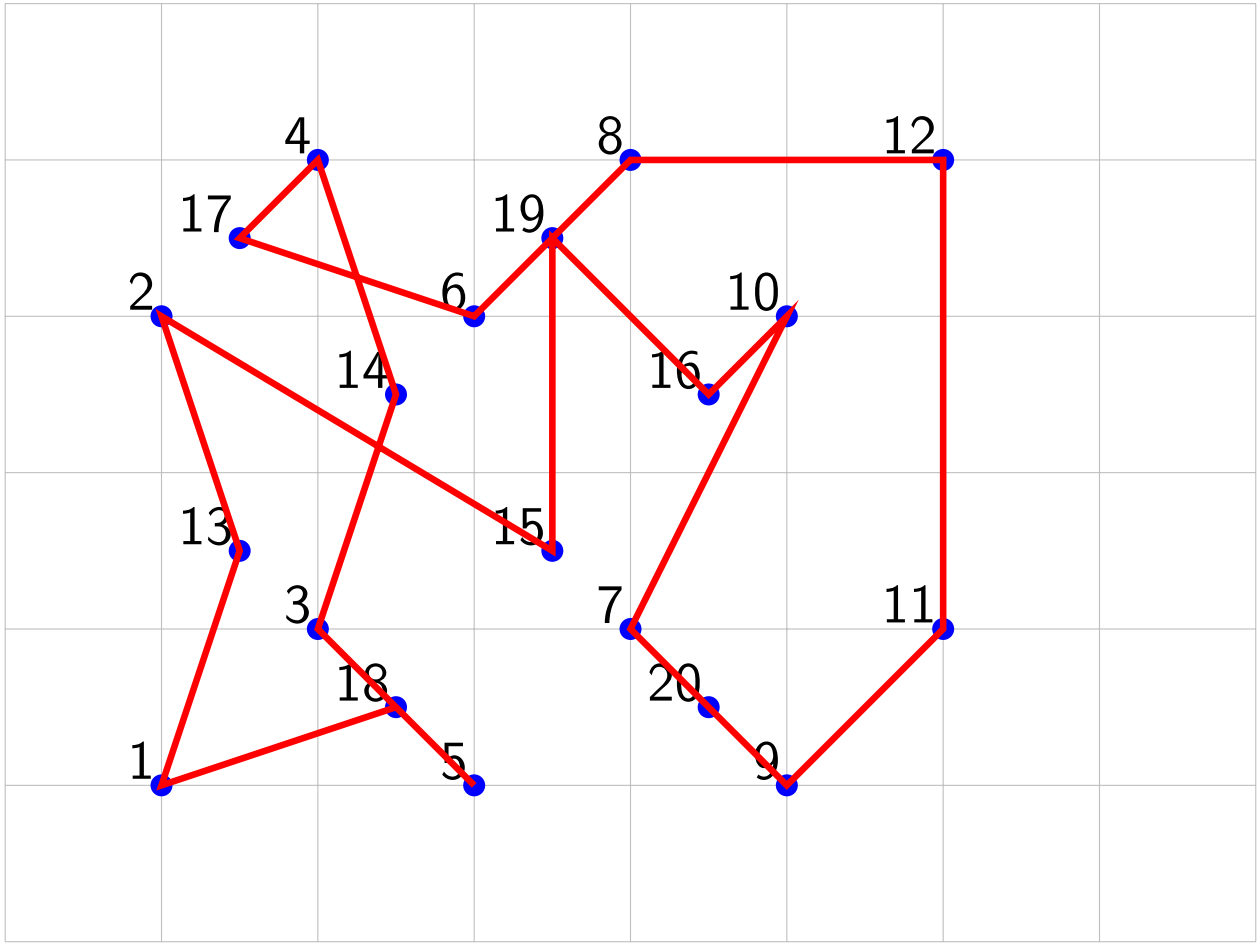
SA Example

$\mathcal{T}_k = 124.94$



SA Example

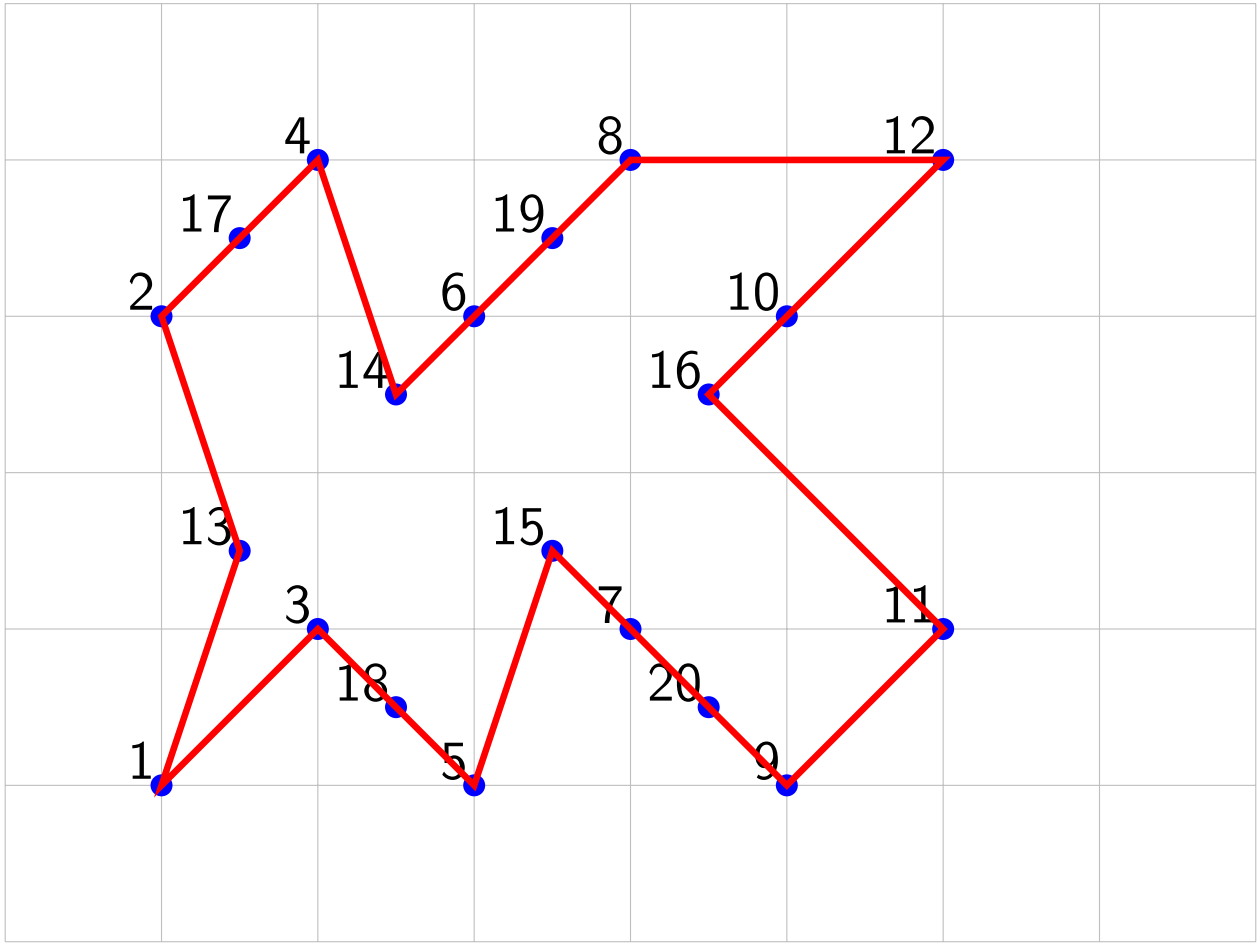
$\mathcal{T}_k = 1.0$



SA Example

$\mathcal{T}_k \simeq 0.0$

Total cost 22.467



SA calibrating parameters

Cooling temperature

- If the cooling factor "α" is to small the temperature will cool down too quickly. The solution might get stuck in local optima;
- If it is too high the algorithm will take longer to converge to a solution.

Temperature

- If the initial temperature is too low, SA can fail to escape local optima.
- If the temperature is too high, SA will take a long time to converge to a solution.

Stopping criteria

- If the stopping criteria is too high, SA will stop before final improvements can be explored.
- If it is too low it might take a long time for the algorithm to stop, even after finding a good solution. There will be no improvements.

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SA calibrating parameters

The cooling:

$$\mathcal{T}_{k+1} = \alpha \times \mathcal{T}_k$$

The algorithm will stop when: $\mathcal{T}_k \leq stop$ **therefore:**

$$\alpha^{k^*} \mathcal{T}_0 = stop$$

Where k^* is the total number of iterations and stop is the stopping value for the temperature.

SA calibrating parameters

To solve for α:

$$\alpha = \left(\frac{\text{stop}}{\mathcal{T}_0}\right)^{\frac{1}{k^*}}$$

To solve for k^*:

$$k^* = \frac{\ln\left(\frac{\text{stop}}{\mathcal{T}_0}\right)}{\ln(\alpha)}$$

To solve for $\mathcal{T}_0$:

$$\mathcal{T}_0 = \frac{\text{stop}}{\alpha^{k^*}}$$

To solve for stop:

$$\text{stop} = \alpha^k \cdot \mathcal{T}_0$$

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SA: Initial Temperature

1. Set stopping criteria "stop" equal to a small number, e.g., $stop = 10^{(-8)}$.

2. Set temperature to a value that is not too small or too large.
   1. Run 20 iterations of the algorithm with the temperature equal to 0, i.e., $\mathcal{T}_0 = 0$;
   2. Determine the absolute value of the difference from the current solution to the new solution;
   3. Set the initial temperature to the average of the difference.

SA: Iterations and cooling rate

It depends how long you have to generate solutions.

1. Determine the time that you have to run the algorithm, e.g., 1 minute, 20 minutes, etc.
2. Determine how long it takes for each iteration and set iterations to the amount of time you have.
3. Set the cooling rate accordingly:

$$\alpha = \left(\frac{\text{stop}}{\mathcal{T}_0} \right)^{\frac{1}{k^*}}$$

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SA: conclusion

- Simulated Annealing is a stochastic algorithm.
- Stochastic algorithms depend on random parameters that change every time we run the algorithm.
- Stochastic algorithms can provide different solutions every time we run.
- It can be necessary to run a few times to get the best solution.

EPFL

Stochastic vs Deterministic

Stochastic algorithms are algorithms that use random elements in their search process. They can be thought of as probabilistic algorithms that make use of randomness to explore the search space.

Deterministic algorithms are algorithms that produce the same output for a given input every time they are run. They do not use any randomness in their search process.

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Summary

- Heuristics are used for the following reasons:
  - When time is of essence;
  - The exact solution might be difficult or impossible to find in a reasonable amount of time;

- It is necessary to have a lower bound to compare the quality of the solutions provided by the heuristic.
  - Heuristic solutions can be arbitrarily bad, while exact methods provide the best solution, heuristics do not.
  - The need to compare and improve the heuristics is always present.

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Summary

Heuristics can be classified in different ways

- **Constructive heuristics:** Build solution from scratch.
  - Nearest Neighbor heuristic.
  - Sorted edges heuristic.
- **Local search**
  - k-opt
- **Deterministic:** if the algorithm converges to the same solution
  - Nearest Neighbor; if we start with a predefined city;
  - Sorted edges
  - k-opt
- **Stochastic:** if the solution depends on some random parameters.
  - Simulated annealing.
  - Nearest Neighbor, if we start in a random city.
- **Greedy:** always choosing the best step:
  - Nearest Neighbor heuristic.
  - Sorted edges heuristic.

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Summary

- Constructive heuristics are fast and can build initial solutions quickly;
- Local search algorithms improve solutions by making specific "moves" that search the neighborhood of the solution;
- Local search heuristics define the neighborhood by the moves;
- Local search heuristics get stuck in local optima and cannot escape;
- To find better solutions we need to escape local optima by momentarily accepting bad solutions that worsen the objective value.
- Simulated Annealing uses a stochastic approach to accept solutions so that there exists a high probability of moving to a worse solution.
- The probability of acceptance of bad solutions decreases as the temperature cools.

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References

- Wolsey, L. A. (1998). *Integer programming*. Wiley.
- Gendreau, M., & Potvin, J.-Y. (Eds.). (2010). *Handbook of metaheuristics*. Springer.